ENERJİ EŞPARÇALANIMI İLE TİTREŞİM SÖNÜMLEMESİ ile ENERJİ GERİ KAZANIMI TEKNİKLERİ GELİŞTİRİLMESİ ÇALIŞMA RAPORU

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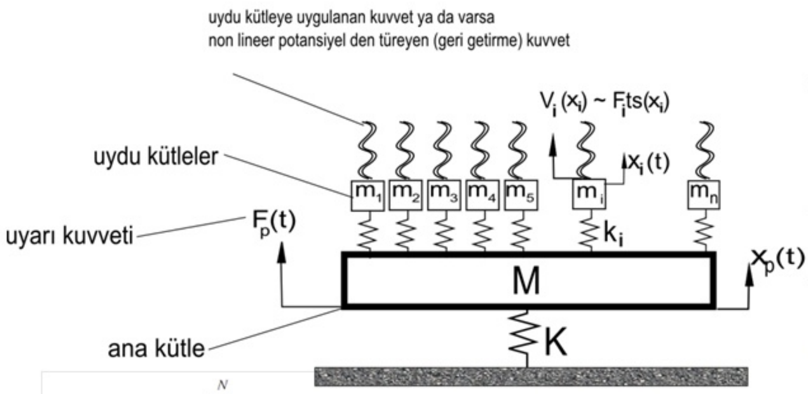
Preparing:

LITERITURE REVIEW

I. Giriş :

Enerji eşparçalanımı metodu, titreşim hareketi yapan ana yapıya fiziksel olarak bağlı farklı özfrekanslara sahip uydu kütlelerin, kendi frekanslarında titreşerek yapıdan titreşim enerjisini her birinde eşit olacak şekilde, kendi üzerilerine çekmeleriyle ana yapıdaki titreşimin enerji çekilerek sönümlendiği metottur.

Enerji geri kazanımındaki temel ilke, uydu kütleler tarafından çekilen enerjinin her bir uydu kütlede sönümlenerek, mekanik enerjiden elektrik enerjisine dönüştürülmesine dayanır.



NonLineer Potansiyel Fonk :
Vi(x)=-Ebond*(-2*exp(-kd*(x-ze))+exp(-2*kd*(x-xe)))

Potansiyelden Türeyen Kuvvet Fonk :
Fts(x)=Ebond*((2*kd)/exp(kd*(x - xe)) - (2*kd)/exp(2*kd*(x - xe)))

avagadro=6.022142*10^23	avagadro sayısı
Ebond=300/avagadro	atomik ağırlık başına enerji (kj)
kd=2.55*10^10	azalma faktörü
ze = 2.42*10^-10	bag mesafesi (m) 2.42 A

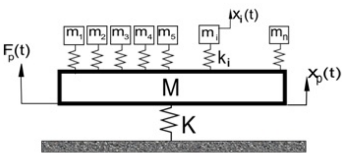
$$Vi(x) = -\mathrm{Ebond}\left(\frac{1}{e^{2\,kd\,(x-xe)}} - \frac{2}{e^{kd\,(x-ze)}}\right)$$

$$M\ddot{x}_M + K_M x_M + \sum_{i=1}^{N} k_i[x_M - x_i] = \mathrm{Fp}(t)$$

$$m_i\ddot{x}_i + k_i[x_i - x_M] = \mathrm{Fts}\left(xi - x(i+1)\right) - \mathrm{Fts}\left(x(i+1) - xi\right)$$

$$Fts(x) = \mathrm{Ebond}\left(\frac{2\,kd}{e^{kd\,(x-xe)}} - \frac{2\,kd}{e^{2\,kd\,(x-xe)}}\right)$$

Lineer Frekans Dağılımı :

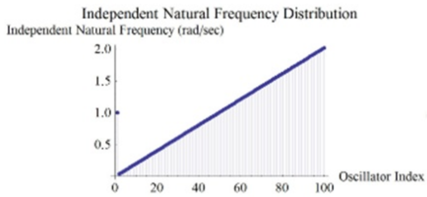


Fp(t) = 0	Ana kütle uyarı giriş kuvveti
xp(0)=1	Ana kütle ilk konumu
x'p(0)=0	Ana kütle ilk hızı
xi(0)=0	Uydu kütle ilk konumları
x'i(0)=0	Uydu kütle ilk hızları

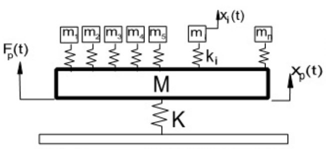
n = 99	Uydu kütle adedi
M = 1 kg	Ana kütle kütle değeri
K = 1 N/m	Ana kütle yay sabiti
mi = 0.1 M/n	Uydu kütle kütle değerleri
wi = 2n/i 0~2 Hz	Uydu kütle frekans değerleri
ki =wi^2 * mi	Uydu kütle yay sabiti

$$M\ddot{x}_M + K_M x_M + \sum_{i=1}^{N} k_i[x_M - x_i] = 0,$$

$$m_i\ddot{x}_i + k_i[x_i - x_M] = 0,$$



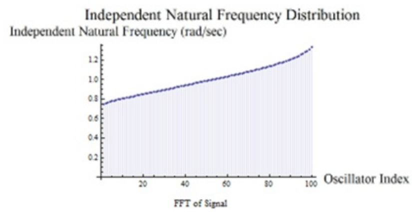
Optimum Frekans Dağılımı :



Fp(t) = 0	Ana kütle uyarı giriş kuvveti
xp(0)=1	Ana kütle ilk konumu
x'p(0)=0	Ana kütle ilk hızı
xi(0)=0	Uydu kütle ilk konumları
x'i(0)=0	Uydu kütle ilk hızları

n = 99	Uydu kütle adedi
M = 1 kg	Ana kütle kütle değeri
K = 1 N/m	Ana kütle yay sabiti
mi = 0.1 M/n	Uydu kütle kütle değerleri
ki =wi^2 * mi	Uydu kütle yay sabiti

wi -> Uydu kütle frekans değerleri



2. Analitik Hesap Yöntemi

MDOF HESAP AKIŞI

m – mass array → M → mass matrix
k – stiffness array → K → stiffness matrix

$x(K - \lambda M) = 0 \rightarrow U, \; [\omega_i]$

$E_{TOP} = \frac{1}{2}\dot{q}^T M \dot{q} + \frac{1}{2} q^T K q$

$q = U\eta$

$U_m = \frac{U}{\sqrt{U^T M U}}$ → mass normalization

$$\boxed{\begin{aligned} L &= T - V = \tfrac{1}{2}\left(\dot{q}^T M \dot{q} - q^T K q\right) \\ \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} &= M\ddot{q} + Kq = 0 \end{aligned}}$$

$E_{\substack{\text{kinetik} \\ \text{satellites}}} = \left\{\frac{1}{2} m_2 \dot{q}_2^2 + \frac{1}{2}(k_i - k_1)^2 q_2^2 + \cdots\right\} -$

Verification

$U_m^T K U_m = [\omega_i^2]$

$U_m^T M U_m = I$

$q = q_h + q_p$

$q_h = \sum_{r=1}^{n}\left[U_m^T M q(0) \cos \omega_r t + \frac{1}{\omega_r} U_m^T M \dot{q}(0) \sin \omega_r t\right] U_m$ * Homojen Çözüm

$q_p = \sum_{r=1}^{n}\left[\frac{U_m^T}{\omega_r}\int_0^t Q(t-\tau) \sin \omega_r \tau \, d\tau\right] U_m$ Partiküler Çözüm

$E_{MODAL} = \dot{\eta}^2 + [\omega_i^2]\eta$

Excitation Force $\underline{Q}(t) = \underline{\theta}_0 \cos \alpha t$

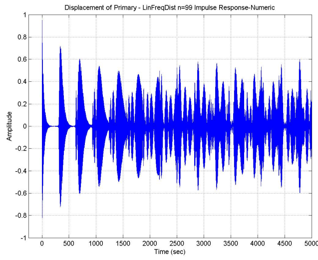
$E_{ERROR} = E_{TOT} - E_{IMP} - E_{QIN}$

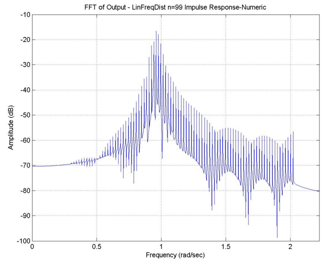
$E_{IMP} = \frac{1}{2}\left(\dot{q}(0)^T M \dot{q}(0) + q(0)^T K q(0)\right)$

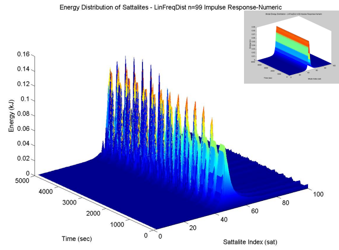
$E_Q = \int \underline{Q}\,\dot{q}(t)\,dt$ constant için $E_{IN_Q}(1) = 0$ olmalı

3. Impulse Response Simulation Results

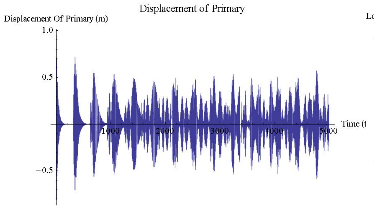
Lineer F.D.
Impulse Response
Numeric Solution

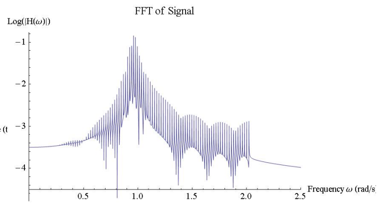


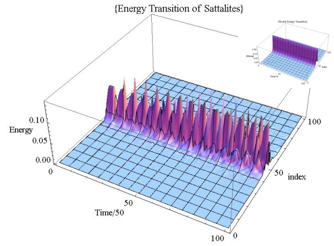




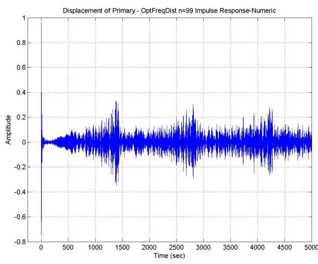
Lineer F.D.
Impulse Response
Analytic Solution

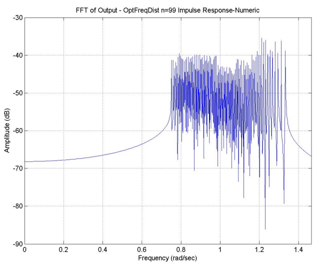


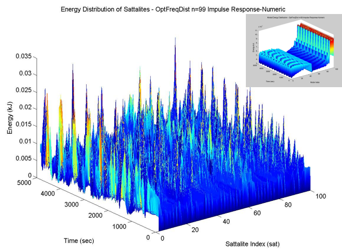




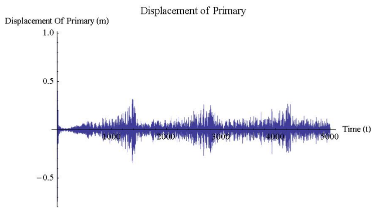
Optimum F.D.
Impulse Response
Numeric Solution

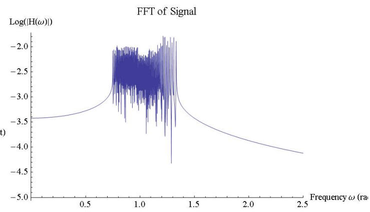


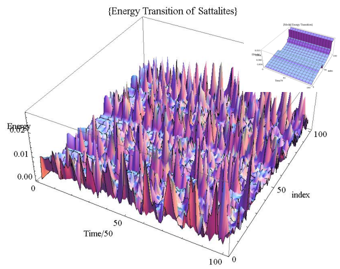




Optimum F.D.
Impulse Response
Analytic Solution



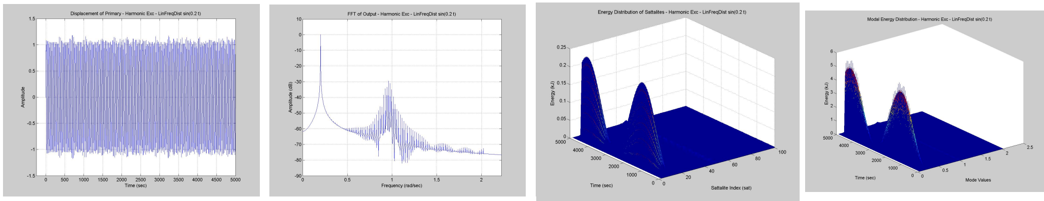




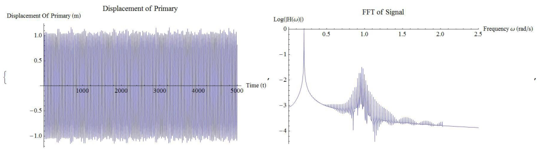
4.1 Harmonic Response of Lineer Freq. Dist.

Sin (0.2 t)

Numeric Solution

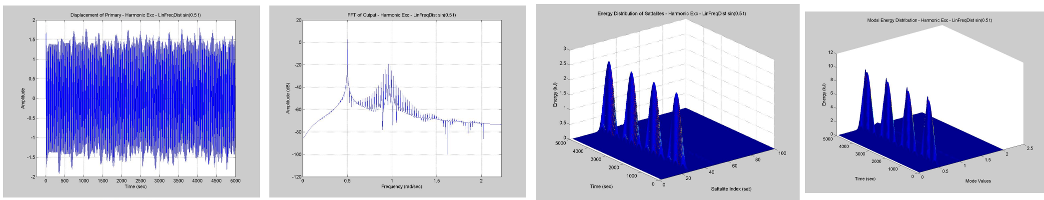


Analytic Solution

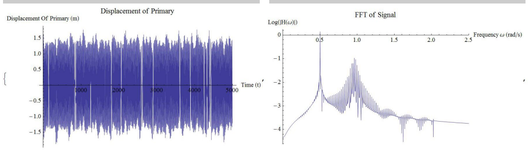


Sin (0.5 t)

Numeric Solution

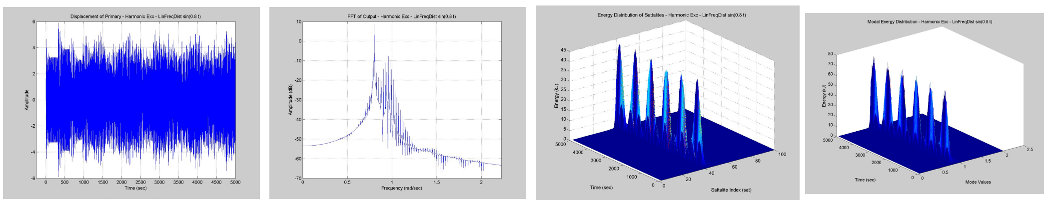


Analytic Solution

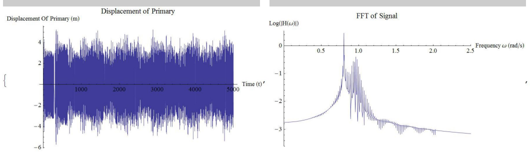


Sin (0.8 t)

Numeric Solution

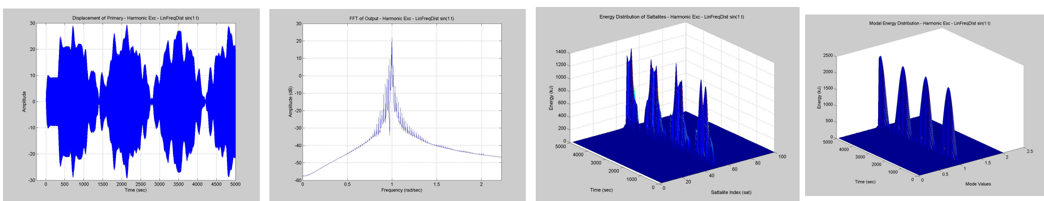


Analytic Solution

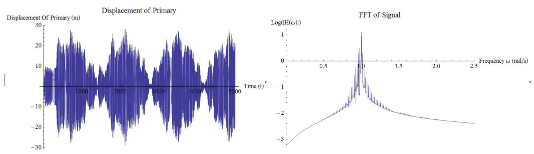


Sin (1 t)

Numeric Solution

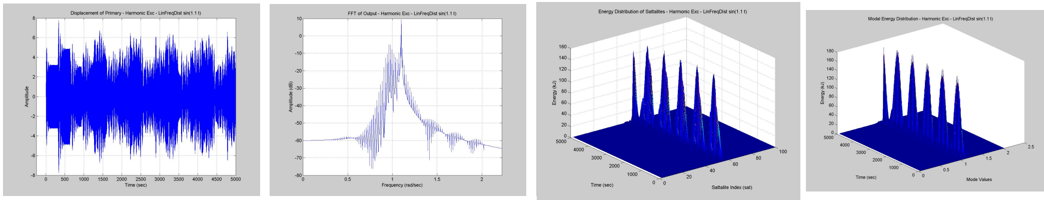


Analytic Solution

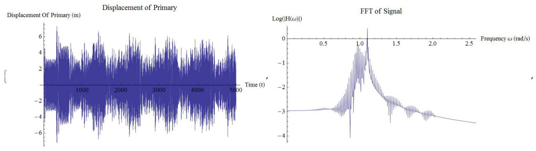


Sin (1.1 t)

Numeric Solution

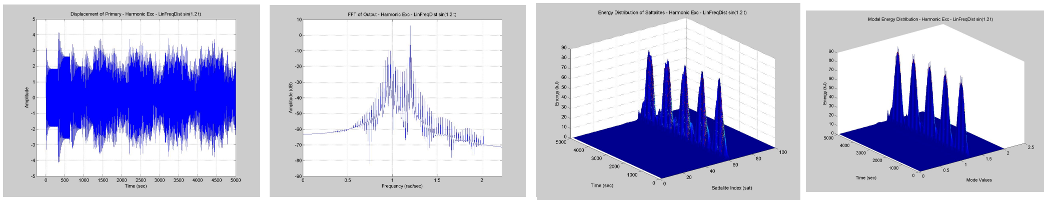


Analytic Solution

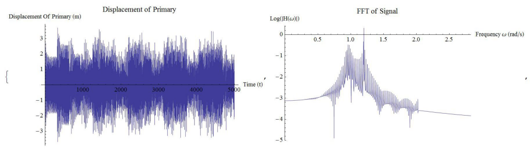


Sin(1.2 t)

Numeric Solution

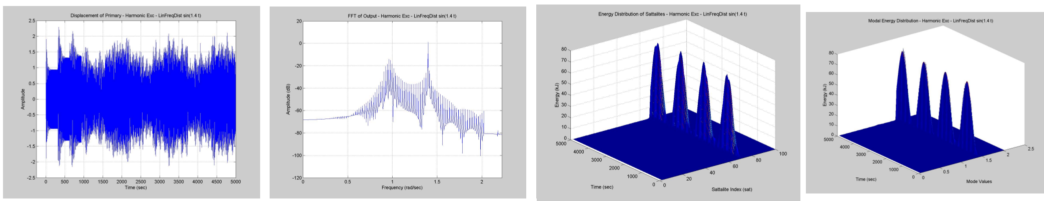


Analytic Solution

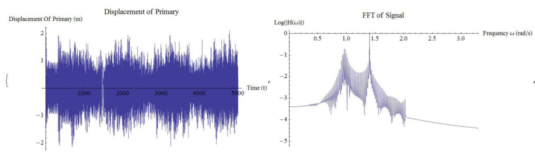


Sin (1.4 t)

Numeric Solution

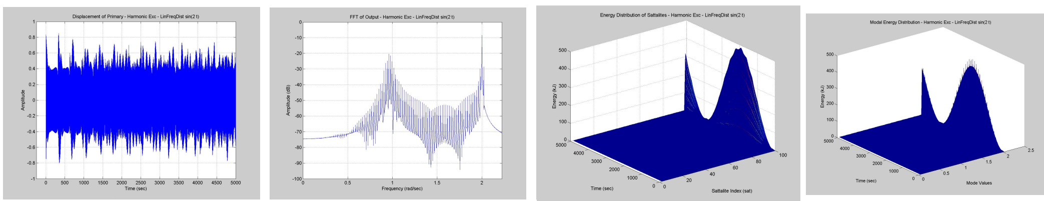


Analytic Solution

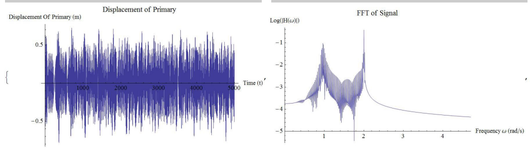


Sin (2 t)

Numeric Solution

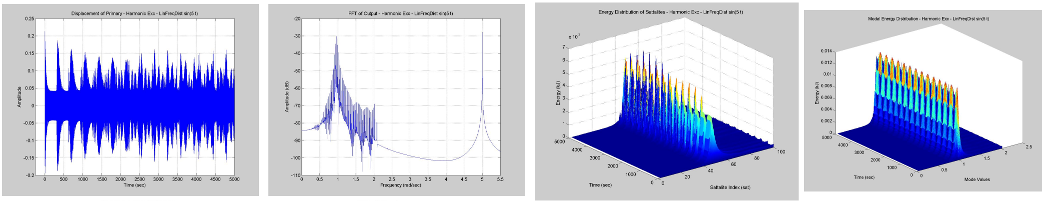


Analytic Solution

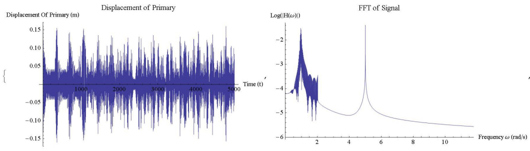


Sin (5 t)

Numeric Solution

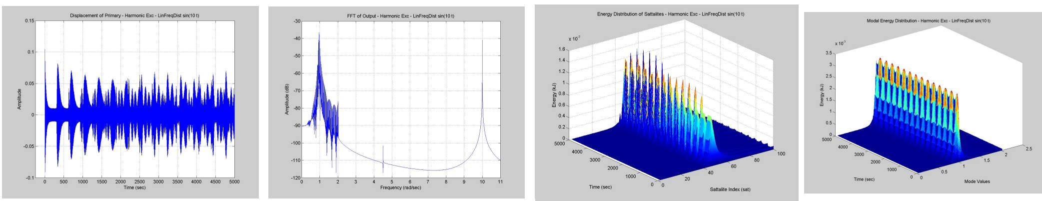


Analytic Solution

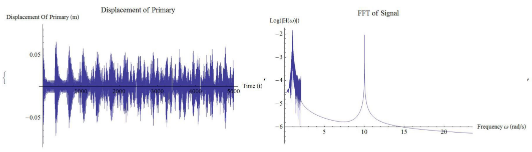


Sin (10 t)

Numeric Solution

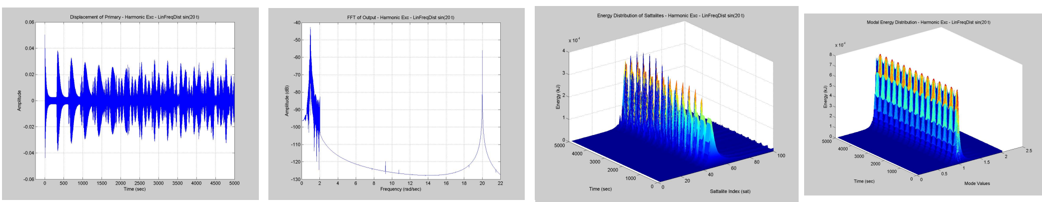


Analytic Solution

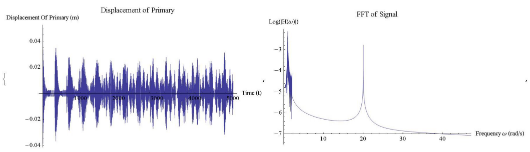


Sin (20 t)

Numeric Solution



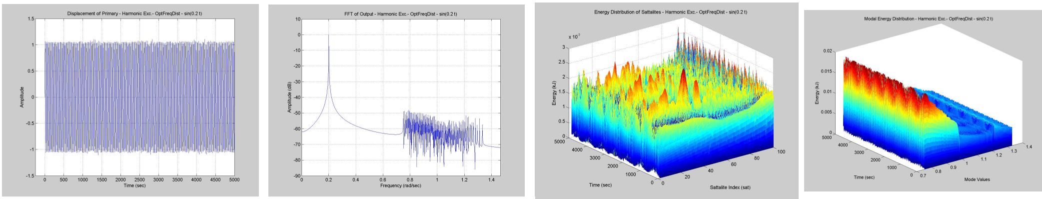
Analytic Solution



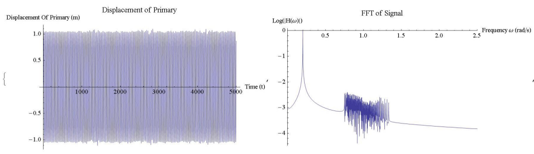
4.2 Harmonic Response of Opt. Freq. Dist.

Sin (0.2 t)

Numeric Solution

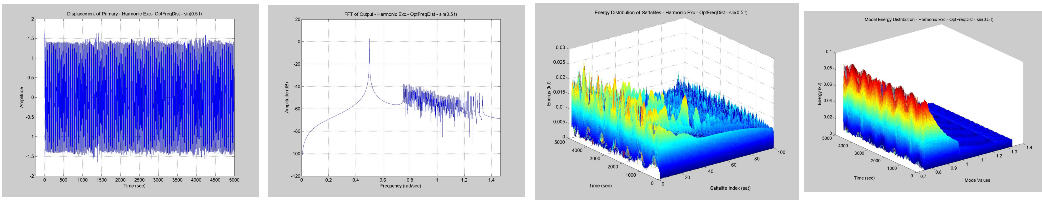


Analytic Solution

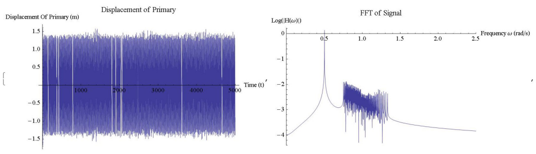


Sin (0.5 t)

Numeric Solution

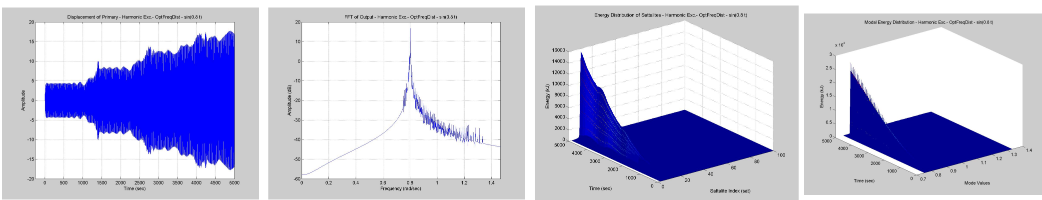


Analytic Solution

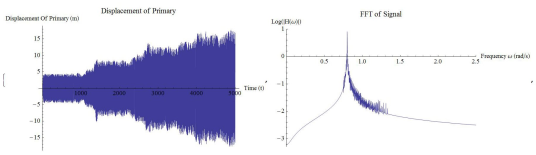


Sin (0.8 t)

Numeric Solution

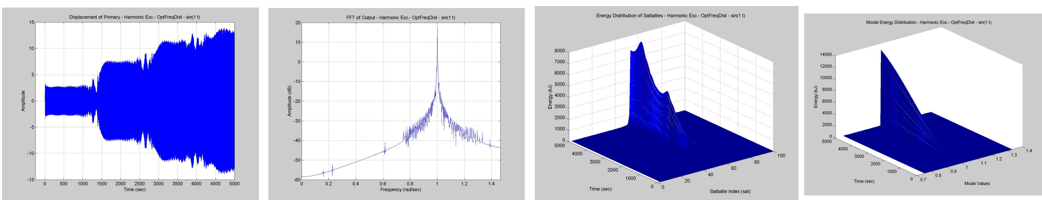


Analytic Solution

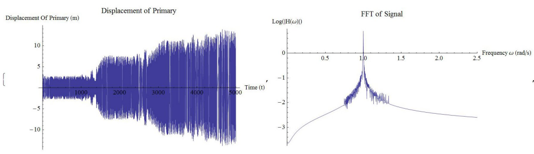


Sin (1 t)

Numeric Solution

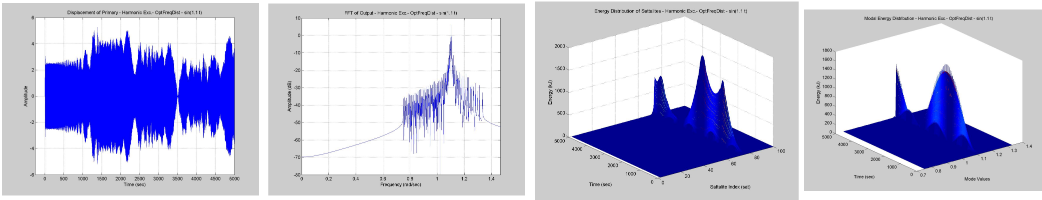


Analytic Solution



Sin (1.1 t)

Numeric Solution



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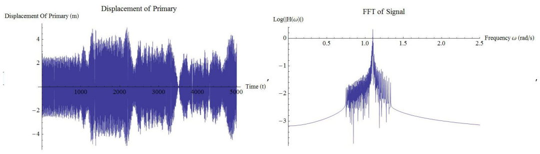
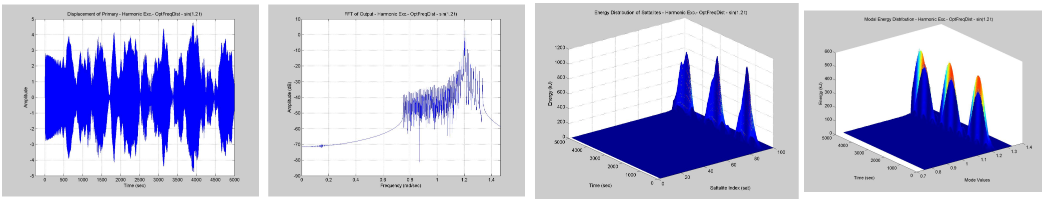
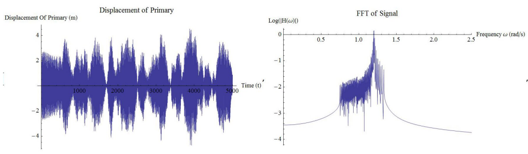


Sin(1.2 t)

Numeric Solution

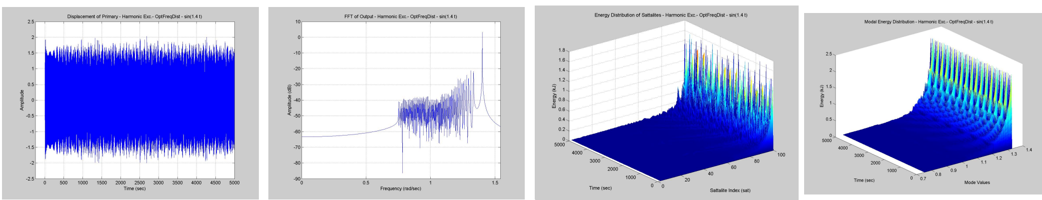


Analytic Solution

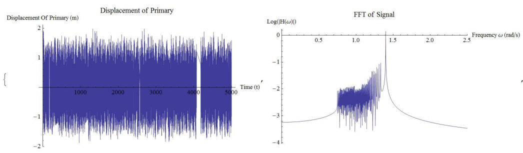


Sin (1.4 t)

Numeric Solution

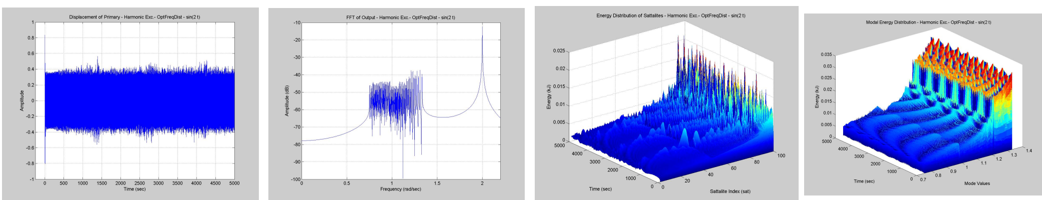


Analytic Solution

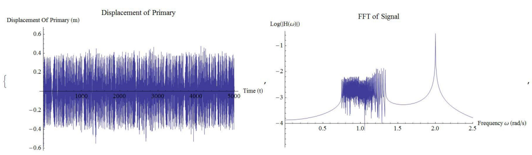


Sin (2 t)

Numeric Solution

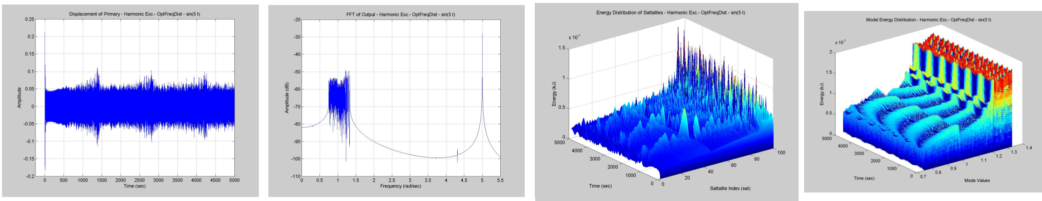


Analytic Solution

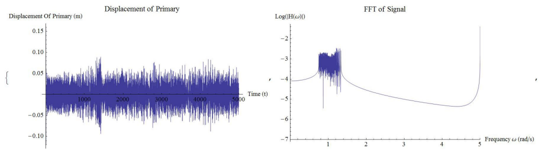


Sin (5 t)

Numeric Solution

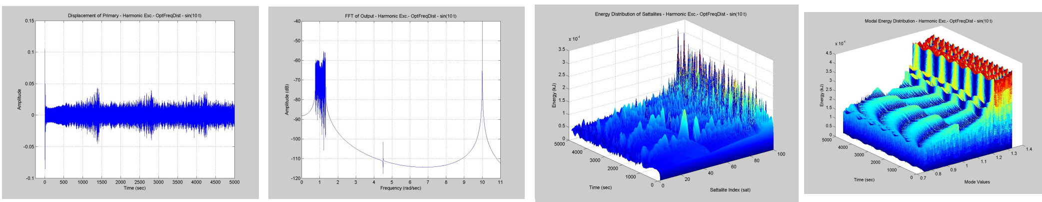


Analytic Solution

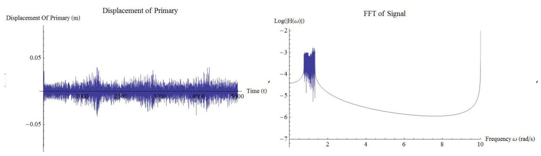


Sin (10 t)

Numeric Solution

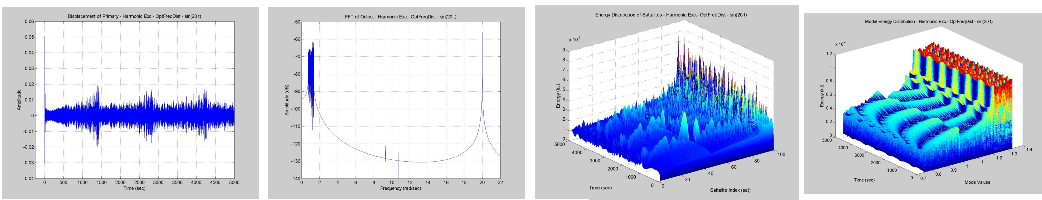


Analytic Solution

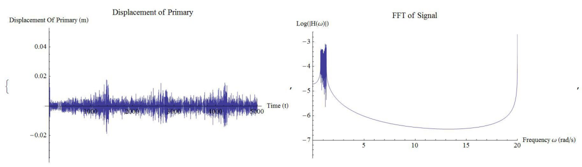


Sin (20 t)

Numeric Solution



Analytic Solution

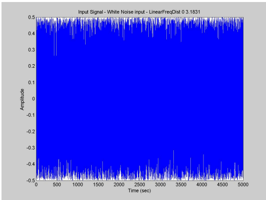
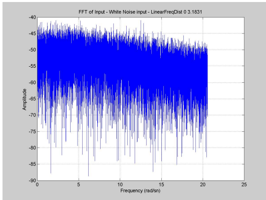


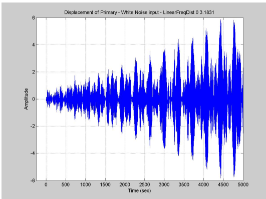
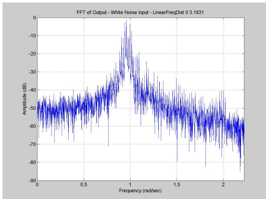
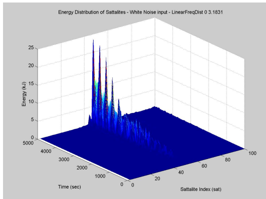
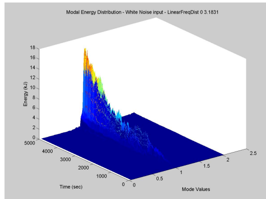
5. White Noise Input to Lin And Opt Freq Dist

Lineer Freq Dist

White Noise

0-20 rad/sec

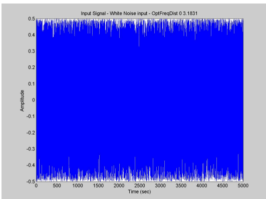
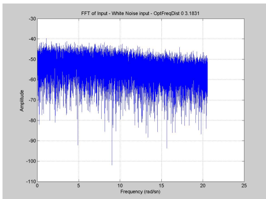



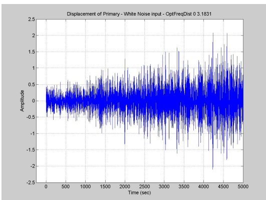
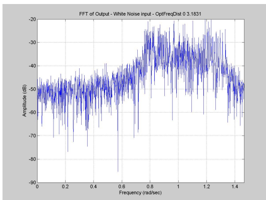
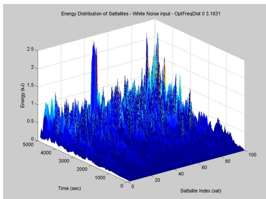
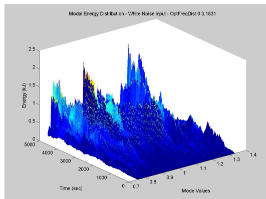





Optimum Freq Dist

White Noise

0-20 rad/sec

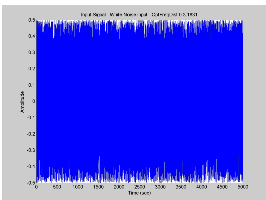
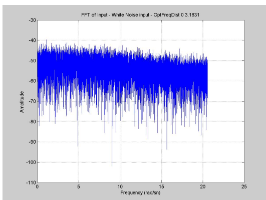



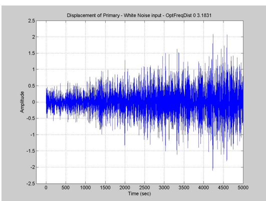
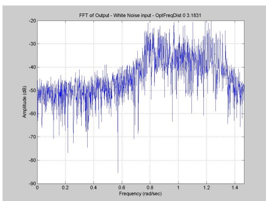
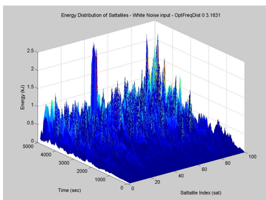
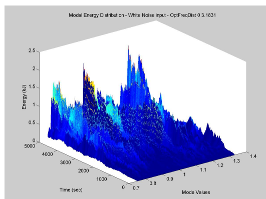





Optimum Freq Dist

White Noise

0-1.34 rad/sec

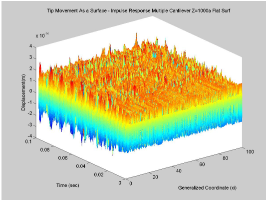





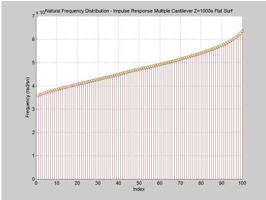
6. Impulse Response - Optimum Frequency Scaled to AFM Frequencies

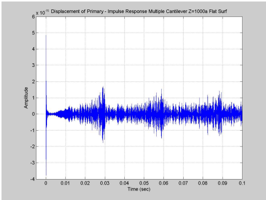
Impulse Response

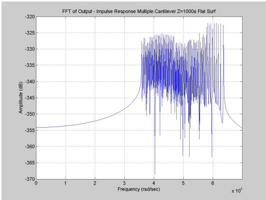
Scaled Opt

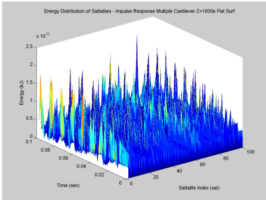
Z=-1000*a

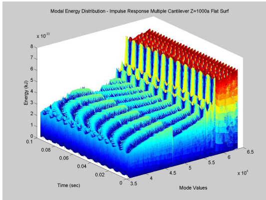












Appendix

A0. Summary OF MDOF Systems

(22-24)/06/10
Gediz

$\underline{M}\ddot{q}(t) + \underline{C}\dot{q}(t) + \underline{K}q(t) = \underline{Q}(t) \rightarrow M = M^T \quad C = C^T \quad K = K^T$ symetric

↳ General form of equations, derived from Lagrangian mechanics.

Influence coefficients

Stiffness inf. coeffs $F_i = \sum_{j=1}^{n} k_{ij} u_j$ — j. den birim deplasman uygulandığında i, yi sabit tutacak (deplasmansız) kuvvet

Flexibility inf. coeffs $u_i = \sum_{j=1}^{n} a_{ij} F_j$ — j. den birim kuvvet girildiğinde, i. deki deplasman.

$A = [a_{ij}] \quad K = [k_{ij}]$

$\underline{A} \cdot \underline{K} = I$

$V = \frac{1}{2} u^T K u \rightarrow$ potansiyel enerji quadratik Formda

$T = \frac{1}{2} u^T M u \rightarrow$ kinetik enerji quadratik Formda

$\mathcal{F}$ or $D = \frac{1}{2} q^T C q \rightarrow$ dissipasyon enerjisi

$$\underbrace{\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_k}\right) - \frac{\partial T}{\partial q_k} + \frac{\partial V}{\partial q_k} + \frac{\partial D}{\partial \dot{q}_k} = Q_k}_{\text{Lagrangian Mechanics}}$$

MODAL Uzayda

$q(t) = U\eta(t) \quad , \quad \ddot{q}(t) = U\ddot{\eta}(t)$

Burda $U \rightarrow$ özvektörler aslında bir (modal uzaya geçişte) transformasyon matrisi olarak da adlandırılır.

$M\ddot{q}(t) + Kq(t) = Q(t) \rightarrow M'\ddot{\eta}(t) + K'\eta(t) = N(t)$

$N(t) = U^T Q(t)$

$M' = U^T M U = M'^T \rightarrow ?$

$K' = U^T K U = K'^T \rightarrow ?$

mass normalisation ?

$$\eta = \begin{pmatrix} C_1 \cos(\omega_1 t - \varphi_1) \\ C_2 \cos(\omega_2 t - \varphi_2) \end{pmatrix} \quad \ddot{\eta} = [\omega_r] \cdot \eta$$

*Burdaki M' ve K' matrisleri modal uzaydaki stiffness ve mass matrisleridir.

Şimdi öyle bir U bulalım ki bu M' ve K' yı sırasıyla inertially ve elastically uncoupled yapsın. Böylece

Böyle bir U matrisi vardır adı modal matristir ve doğal modları içerir.

$M'_{jj}\ddot{\eta}_j(t) + K'_{jj}\eta_j(t) = N_j(t)$ olsun.

↳ independent equations are reffered as modal equations.

↳ solution of these diffeqs called modal analysis

* Eğer U M' ve K' 'i diagonal yapacak bir matris ise ikisine göre de ortogonaldir

Eğer $\tilde{M}'$ i ben I yaparsam normalizasyon yapmış oluyorum.

ORTHOGONALITY of MODAL VEC.

$u_s^T K u_r = \omega_r^2 u_s^T M u_r$

$u_r^T K u_s = \omega_s^2 u_r^T M u_s$

$K u_r = \omega_r^2 M u_r \sim K u_s = \omega_s^2 M u_s \leftarrow x = q = U\eta = \{\bar{u}_1, \bar{u}_2, \bar{u}_3\}\eta \rightarrow Kx + M\ddot{x} = 0$

$KU\eta\,[\omega_i]^2 MU\eta = 0$?

↳ * Zaten modal koordinatlara geçiş kütle ve yay matrislerini decoupled hale getirmekti (modal coordinatlar cinsinden) öyleyse modal vektörle çarpınca elime doğal frekans n. mod'un gelmesi de anlaşılır bir durum

A.1 Summary Of Calculations MDOF System

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) - \frac{\partial L}{\partial x_i} = Q_{(i)}^{nc} \longrightarrow M\ddot{x} + Kx = Q \longrightarrow x(K - \lambda M) = 0$$

$$\lambda = \omega^2 \longrightarrow [\cdot\omega_i^2\cdot]$$

$$\eta = U^{-1} \cdot x \qquad \tilde{K} = U^T K U \qquad \tilde{M} = U^T M U \qquad N(t) = U^T Q(t)$$

modal disp — modal stiffness — modal Mass — modal Forces

$$M\ddot{x} + Kx = Q$$

$$\eta\left(-\lambda U^T M U + U^T K U\right) = U^T Q$$

$$\eta\left(-\underbrace{\lambda}_{[\cdot\omega_i^2\cdot]} \tilde{M} + \tilde{K}\right) = \tilde{N} \longrightarrow \eta\left(-[\cdot\omega_i^2\cdot]\underbrace{\tilde{M}}_{I} + \underbrace{\tilde{K}}_{[\cdot\omega_i^2\cdot]}\right) = \tilde{N}$$

Aynı şekilde Emodal

$$E_{TOP} \in D[x] \rightarrow E_{modal} \in D[\eta] \quad E_A = \frac{1}{2}\eta^2\left(-U^T M U [\cdot\omega_i^2\cdot] + U^T K U\right) \longrightarrow \frac{1}{2}\eta\left(-[\cdot\omega_i^2\cdot]\underbrace{\tilde{M}}_{I} + \underbrace{\tilde{K}}_{[\cdot\omega_i^2\cdot]}\right)$$

$$E_{modal} = \frac{1}{2}\left(\dot{\eta}^2 + [\cdot\omega_i^2\cdot]\,\eta^2\right) \longrightarrow$$ buradan ayrık (diagonalize edilmiş) sistemde

$$E_{i_{modal}} = \frac{1}{2}\left(\dot{\eta}_i^2 + \omega_i^2 \eta_i\right) \longrightarrow$$ i. moddaki enerji

$$E_{modal_i} = \frac{1}{2} C_i^2 \omega_i^2$$

ANALİTİK ÇÖZÜM:

$$\eta_r(t) = C_r \cos(\omega_r t - \varphi_r) = \underbrace{\eta_r(0)}_{{}^aC_r} \cos(\omega_r t) + \underbrace{\frac{\dot{\eta}_r(0)}{\omega_r}}_{{}^bC_r} \sin \omega_r t$$

Modal initial Conditions

$$(U^T M U) \longrightarrow$$ eğer mass normalize etmezsen α^2 veriyor.

$$C_r = \sqrt{{}^aC_r^2 + {}^bC_r^2}$$

$$\varphi_r = \arctan\left(\frac{-{}^bC_r}{{}^aC_r}\right)$$

böylece $$q(t) = \sum_{r=1}^{n}\left(u_r^T M q(0) \cos \omega_r t + \frac{1}{\omega_r} u_r^T M \dot{q}(0) \sin \omega_r t\right) u_r$$

A.2 Example Problem (Validation of Operator and Function use in Mathematica)

"CONTENT"

"*Mathematica* Built-in Function Test using a problem which has a known solution
- Meireovitch // Fundementals of Vibration //Two Degree Of Freedom Systems//Example 5.2//Page 221"

"Question"

Example 5.2. Consider the simplified model of an automobile shown in Fig. 5.5, let the parameters have the values $m = 1,500$ kg, $I_C = 2,000$ kg m^2, $k_1 = 36,000$ kg/m, $k_2 = 40,000$ kg/m, $a = 1.3$ m and $b = 1.7$ m, calculate the natural modes of the system and write an expression for the response.

"Equations Of Motion in Matrix Form"

$$\begin{bmatrix} 1,500 & 0 \\ 0 & 2,000 \end{bmatrix}\begin{bmatrix} \ddot{x} \\ \ddot{\theta} \end{bmatrix} + \begin{bmatrix} 76,000 & 21,200 \\ 21,200 & 176,440 \end{bmatrix}\begin{bmatrix} x \\ \theta \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad \text{(a)}$$

But, free vibration is harmonic, so that by analogy with Eqs. (5.23) and (5.31) we can write

$$x(t) = X\cos(\omega t - \phi), \; \theta(t) = \Theta\cos(\omega t - \phi) \qquad \text{(b)}$$

"Results"

$$\mathbf{x}(t) = C_1 \cos(6.857811t - \phi_1)\begin{bmatrix} 1 \\ -0.257341 \end{bmatrix} + C_2 \cos(9.584211t - \phi_2)\begin{bmatrix} 1 \\ 2.914417 \end{bmatrix} \qquad \text{(l)}$$

where the amplitudes C_1, C_2 and the phase angles ϕ_1, ϕ_2 must be determined from the initial displacements $x(0)$, $\theta(0)$ and the initial velocities $\dot{x}(0)$, $\dot{\theta}(0)$, as will be shown in Sec. 5.4.

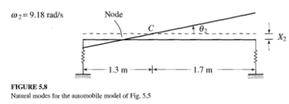


FIGURE 5.8
Natural modes for the automobile model of Fig. 5.5

"Mass Matrix"

$$\begin{pmatrix} 1500. & 0. \\ 0. & 2000. \end{pmatrix}$$

"Stifness Matrix"

$$\begin{pmatrix} 76000. & 21200. \\ 21200. & 176440. \end{pmatrix}$$

"EigenFrequencies"

$\{6.85781, 9.58421\}$

"EigenVectors"

$$\begin{pmatrix} -0.968447 & 0.324548 \\ 0.249221 & 0.945869 \end{pmatrix}$$

"Checking Orthogonality"

3.63798×10^{-12}

"Mass Nomalization Formula"

$$\text{Us2} = \frac{\text{Us}}{\sqrt{\text{Us}.M.\text{Us}}}$$

"Mass Normalized EigenVectors"

$$\begin{pmatrix} -0.0247503 & 0.0073546 \\ 0.00636927 & 0.0214344 \end{pmatrix}$$

"Unit Normalized EigenVectors"

$$\begin{pmatrix} 1. & 1. \\ -0.257341 & 2.91442 \end{pmatrix}$$

A3. Comparision between Analytic Solution and Numeric Solution

$$M = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0.04 & 0 \\ 0 & 0 & 0.06 \end{pmatrix}$$

```
{{1, 0, 0}, {0, 0.04, 0}, {0, 0, 0.06}}
```

$$K = \begin{pmatrix} 1.26 & -0.02 & -0.24 \\ -0.02 & 0.02 & 0 \\ -0.24 & 0 & 0.24 \end{pmatrix}$$

```
{{1.26, -0.02, -0.24}, {-0.02, 0.02, 0}, {-0.24, 0, 0.24}}
```

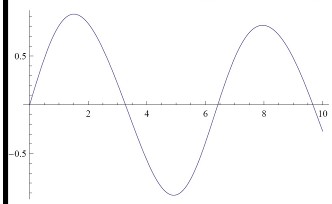
Impulse Response 3DOF System

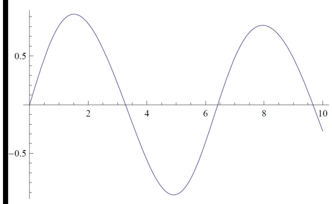
```
"ANALITIK COZUM"
q0 = {0, 0, 0};
dq0 = {1, 0, 0};
q = Sum[
   (Um[[All, i]].M.q0 * Cos[ωi[[i]] * t] + 1 / ωi[[i]] * Um[[All, i]].M.dq0 * Sin[ωi[[i]] * t]) *
    Um[[All, i]] , {i, 1, 3}]
```

```
ANALITIK COZUM

{-0.193239 (0. Cos[0.693019 t] - 0.278837 Sin[0.693019 t]) +
   0.932324 (0. Cos[0.982431 t] + 0.948997 Sin[0.982431 t]) -
   0.305665 (0. Cos[2.07715 t] - 0.147156 Sin[2.07715 t]),
  -4.89838 (0. Cos[0.693019 t] - 0.278837 Sin[0.693019 t]) -
   1.00213 (0. Cos[0.982431 t] + 0.948997 Sin[0.982431 t]) +
   0.0400656 (0. Cos[2.07715 t] - 0.147156 Sin[2.07715 t]),
  -0.219607 (0. Cos[0.693019 t] - 0.278837 Sin[0.693019 t]) +
   1.22883 (0. Cos[0.982431 t] + 0.948997 Sin[0.982431 t]) +
   3.88695 (0. Cos[2.07715 t] - 0.147156 Sin[2.07715 t])}
```

```
"SolutionBySolver"
TIME = 10;

X = {x1[t], x2[t], x3[t]};
D2X = D[X, {t, 2}];
Eqs = {0, 0, 0};

Table[Eqs[[i]] = (M.D2X + K.X)[[i]] == 0, {i, 1, 3}];
Eqs // MatrixForm
vars = {x1, x2, x3}
IC = {x1[0] == 0, x2[0] == 0, x3[0] == 0, x1'[0] == 1, x2'[0] == 0, x3'[0] == 0}
dsol = NDSolve[Flatten[{Eqs, IC}], vars, {t, 0, TIME}, AccuracyGoal → 16,
   PrecisionGoal → 16, Method → "ExplicitRungeKutta", MaxSteps → ∞]
Plot[Evaluate[x1[t] /. %], {t, 0, TIME}]
Plot[q[[1]], {t, 0, TIME}]
Plot[q[[1]] - Evaluate[x1[t] /. dsol], {t, 0, TIME}, PlotRange → All]
```

```
SolutionBySolver

( 1.26 x1[t] - 0.02 x2[t] - 0.24 x3[t] + x1''[t] == 0
   -0.02 x1[t] + 0.02 x2[t] + 0.04 x2''[t] == 0
   -0.24 x1[t] + 0.24 x3[t] + 0.06 x3''[t] == 0 )

{x1, x2, x3}

{x1[0] == 0, x2[0] == 0, x3[0] == 0, x1'[0] == 1, x2'[0] == 0, x3'[0] == 0}

{{x1 → InterpolatingFunction[{{0., 10.}}, <>], x2 → InterpolatingFunction[{{0., 10.}}, <>],
  x3 → InterpolatingFunction[{{0., 10.}}, <>]}}
```



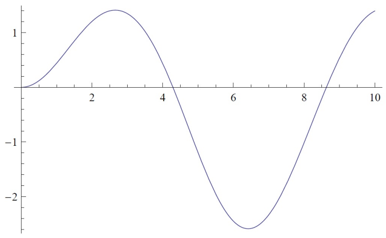


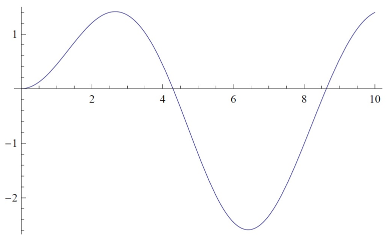
Harmonic Excitation 3DOF System

```
"FOR HARMONIC EXCITATIONS"
Q0 = {1, 0, 0};
α = 0.5;
Q[t_] = Q0 * Cos[α * t];
% // MatrixForm
NF = Table[Um[[All, i]].Q0 * Cos[α * t], {i, 1, 3}];
% // MatrixForm

qharm = Sum[ Um[[All, i]] / ωi[[i]] *
     Integrate[Q[t - τ] * Sin[ωi[[i]] * τ], {τ, 0, t}].Um[[All, i]] , {i, 1, 3}];
% // MatrixForm

Plot[qharm[[1]], {t, 0, TIME}]


Table[Eqs[[i]] = (M.D2X + K.X)[[i]] == Q0[[i]] * Cos[α * t], {i, 1, 3}];
IC = {x1[0] == 0, x2[0] == 0, x3[0] == 0, x1'[0] == 0, x2'[0] == 0, x3'[0] == 0};
dsol2 = NDSolve[Flatten[{Eqs, IC}], vars, {t, 0, TIME}, AccuracyGoal → 16,
    PrecisionGoal → 16, Method → "ExplicitRungeKutta", MaxSteps → ∞];
Plot[Evaluate[x1[t] /. dsol2], {t, 0, TIME}]
Plot[qharm[[1]] - Evaluate[x1[t] /. dsol2], {t, 0, TIME}, PlotRange → All]
```

```
FOR HARMONIC EXCITATIONS

( Cos[0.5 t]
      0
      0     )

( -0.193239 Cos[0.5 t]
   0.932324 Cos[0.5 t]
  -0.305665 Cos[0.5 t] )

( 0.0538821 (3.00952 Cos[0.5 t] - 3.00952 Cos[0.693019 t] + 0. i Sin[0.5 t] + 0. i Sin[0.6930
  1.36585 (3.00952 Cos[0.5 t] - 3.00952 Cos[0.693019 t] + 0. i Sin[0.5 t] + 0. i Sin[0.69301
  0.0612345 (3.00952 Cos[0.5 t] - 3.00952 Cos[0.693019 t] + 0. i Sin[0.5 t] + 0. i Sin[0.693
```

*****





Analytic Solution of Harmonic Excitation 3DOF ***

```
( 0.0538821 (3.00952 Cos[0.5 t] - 3.00952 Cos[0.693019 t] + 0. i Sin[0.5 t] + 0. i Sin[0.693019 t]) + 0.884772 (1.3737 Cos[0.5 t] - 1.3737 Cos[0.982431 t] + 0. i Sin[0.5 t] + 0. i Sin[0.982431 t]) + 0.0449804 (0.51104 Cos[0.5 t] - 0.51104 Cos[2.07715 t] + 0. i Sin[0.5 t] + 0. i Sin[2.07715 t])
  1.36585 (3.00952 Cos[0.5 t] - 3.00952 Cos[0.693019 t] + 0. i Sin[0.5 t] + 0. i Sin[0.693019 t]) - 0.95102 (1.3737 Cos[0.5 t] - 1.3737 Cos[0.982431 t] + 0. i Sin[0.5 t] + 0. i Sin[0.982431 t]) - 0.00589589 (0.51104 Cos[0.5 t] - 0.51104 Cos[2.07715 t] + 0. i Sin[0.5 t] + 0. i Sin[2.07715 t])
  0.0612345 (3.00952 Cos[0.5 t] - 3.00952 Cos[0.693019 t] + 0. i Sin[0.5 t] + 0. i Sin[0.693019 t]) + 1.16616 (1.3737 Cos[0.5 t] - 1.3737 Cos[0.982431 t] + 0. i Sin[0.5 t] + 0. i Sin[0.982431 t]) - 0.571988 (0.51104 Cos[0.5 t] - 0.51104 Cos[2.07715 t] + 0. i Sin[0.5 t] + 0. i Sin[2.07715 t]) )
```

A.4 Calculation of Modal Coordinates and Energies

"Analytic Solution of Generalized and Modal Coordinates"

$$\eta h = \mathrm{Table}\left[\frac{\sin(t\,\Omega t[[i]])\,\{\mathrm{Umt}[[\mathrm{All},i]]\}.\mathrm{Mt.dq0t}}{\Omega t[[i]]} + \cos(t\,\Omega t[[i]])\,\{\mathrm{Umt}[[\mathrm{All},i]]\}.\mathrm{Mt.q0t},\ \{i,1,\mathrm{nt}\}\right];$$

$$\mathrm{qh} = \sum_{i=1}^{\mathrm{nt}} \eta h[[i]].\{\mathrm{Umt}[[\mathrm{All},i]]\};$$

$$\mathrm{Nf} = \mathrm{Table}[\{\mathrm{Umt}[[\mathrm{All},i]]\}.\mathrm{Qt},\ \{i,1,\mathrm{nt}\}];$$

$$\eta p = \mathrm{Table}\left[\frac{\int_0^t \sin(\tau\,\Omega t[[i]])\,(\mathrm{Nf}[[i]]\ /.\ t \to t-\tau)\,d\tau}{\Omega t[[i]]},\ \{i,1,\mathrm{nt}\}\right];$$

$$\mathrm{qp} = \sum_{i=1}^{\mathrm{nt}} \eta p[[i]].\{\mathrm{Umt}[[\mathrm{All},i]]\};$$

"Analytic Solution of Energies"

$$\mathrm{System(EperSat)} = \mathrm{Table}\left[0.5\left(\mathrm{kt}[[i]]\,(\mathrm{qt}[[i]]-\mathrm{qt}[[1]])^2 + \mathrm{mt}[[i]]\,\mathrm{qdot}[[i]]^2\right),\ \{i,2,\mathrm{nt}\}\right];$$

$$\mathrm{System(ETot)} = 0.5\,(\mathrm{qt.Kt.qt} + \mathrm{qdot.Mt.qdot});$$

$$\mathrm{EForcet} = \int \mathrm{Qt.qdot}\,dt;$$

$$\mathrm{EF0} = \mathrm{EForcet}\ /.\ t \to 0;$$

$$\mathrm{System(EForce)} = \mathrm{EForcet} - \mathrm{EF0};$$

$$\mathrm{System(EModal)} = \mathrm{Table}\left[0.5\left(\eta\mathrm{dot}[[i]]^2 + \eta t[[i]]^2\,\Omega t[[i]]^2\right)[[1]],\ \{i,1,\mathrm{nt}\}\right];$$

$$\mathrm{System(EImp)} = 0.5\,(\mathrm{dq0t.Mt.dq0t} + \mathrm{q0t.Kt.q0t}) + \mathrm{System(EForce)};$$

Umt - Mass Normalized Eigen Vectors

etah - homogenous solution eta

etap - particular solution eta

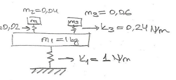
Nf - modal forces transposed from generalized forces

qp - particular solution

qh - homogenous solution

Look at A1 All Explained clearly

A.5 Energy Check for Impulse Response (Time independent modal energy distribution).



Elle yapılanları kontrol

$m_2=0{,}04$ $m_3=0{,}06$ $k_2=0{,}02$ $k_3=0{,}24$ N/m $m_1=1$ kg $k_1=1$ N/m

```
In[1]:= M = {{1, 0, 0}, {0, 0.04, 0}, {0, 0, 0.06}}   M
Out[1]= {{1, 0, 0}, {0, 0.04, 0}, {0, 0, 0.06}}
In[2]:= K = {{1.26, -0.02, -0.24}, {-0.02, 0.02, 0}, {-0.24, 0, 0.24}}   K
Out[2]= {{1.26, -0.02, -0.24}, {-0.02, 0.02, 0}, {-0.24, 0, 0.24}}
In[3]:= Inverse[M] // MatrixForm
Out[3]//MatrixForm= {{1., 0., 0.}, {0., 25., 0.}, {0., 0., 16.6667}}   M^-1
In[4]:= Inverse[M].K // MatrixForm
Out[4]//MatrixForm= {{1.26, -0.02, -0.24}, {-0.5, 0.5, 0.}, {-4., 0., 4.}}   M^-1 K
In[5]:= Inverse[M].K - λ {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}};   (M^-1 K - λ) Eigenvalue prob.
        % // MatrixForm
Out[6]//MatrixForm= {{1.26 - λ, -0.02, -0.24}, {-0.5, 0.5 - λ, 0.}, {-4., 0., 4. - λ}}  → (M^-1 K - λ)
In[7]:= Det[%]
        Solve[% == 0]
        ωn = λ /. %
Out[7]= 2. - 6.7 λ + 5.76 λ^2 - λ^3   → karakteristik denk det|(M^-1 K - λ)|
Out[8]= {{λ → 0.480275}, {λ → 0.96517}, {λ → 4.31455}}   → λ1,2,3
Out[9]= {0.480275, 0.96517, 4.31455}   → {ωi^2}
```

* ÖRNEK PROBLEM ÜZERİNDEN DECOUPLING MODAL TRANSFORMASYON - MODAL ENERJİ KAVRAMI 'nın sonuca bağlanma çalışması.

```
In[10]:= esys = Eigensystem[Inverse[M].K];
         U = Transpose[Reverse[esys[[2]]]];
         ω2e = Reverse[esys[[1]]];
         ω2 = {{%[[1]], 0, 0}, {0, %[[2]], 0}, {0, 0, %[[3]]}};
         % // MatrixForm
         U // MatrixForm
         Um = U;
         Table[
           Um[[All, i]] = U[[All, i]] / Sqrt[ U[[All, i]].M.U[[All, i]] ]
           , {i, 1, 3}];
         Um // MatrixForm
Out[14]//MatrixForm= {{0.480275, 0, 0}, {0, 0.96517, 0}, {0, 0, 4.31455}}   → [ωi^2]
Out[15]//MatrixForm= {{-0.0393794, 0.506853, -0.0783925}, {-0.998222, -0.544804, 0.0102754}, {-0.0447528, 0.668048, 0.99687}}   → U (özvektörler)
Out[18]//MatrixForm= {{-0.193239, 0.932324, -0.305665}, {-4.89838, -1.00213, 0.0400656}, {-0.219607, 1.22883, 3.88695}}   → Kütle normalize özvektörler Um
Mm = Round[Transpose[U].M.U, 0.00000000000001];
% // MatrixForm
Km = Round[Transpose[U].K.U, 0.00000000000001];
% // MatrixForm
```

Modal Transformasyona uğramış Kütle ve Yay matrisleri

```
Out[20]//MatrixForm= {{0.0415288, 0, 0}, {0, 0.29555, 0}, {0, 0, 0.0657746}}   → M' = Mm = U^T M U
Out[22]//MatrixForm= {{0.0199452, 0, 0}, {0, 0.285256, 0}, {0, 0, 0.283788}}   → K' = Km = U^T K U
```

Diagonalize edilmiş (Uncoupling)

```
In[26]:= {Km // MatrixForm, ω2 // MatrixForm, Mm // MatrixForm}
Out[26]= {{{0.0199452, 0, 0}, {0, 0.285256, 0}, {0, 0, 0.283788}},   → Km
          {{0.480275, 0, 0}, {0, 0.96517, 0}, {0, 0, 4.31455}},
          {{0.0415288, 0, 0}, {0, 0.29555, 0}, {0, 0, 0.0657746}}}   → Mm
In[27]:= Km - ω2.Mm // MatrixForm        λ = ω^2
         Round[Det[%], .000000000000001] === 0
Out[27]//MatrixForm= {{2.76515×10^-15, 0., 0.}, {0., 3.33067×10^-15, 0.}, {0., 0., 2.10942×10^-15}}   → Km - λ Mm ≈ 0
Out[28]= True   Km - λMm =? 0
```

(2)

```
In[29]:= True
         "Aynisinin Mass Normalizationla"
         Mm = Round[Transpose[Um].M.Um, 0.00000000000001];
         % // MatrixForm
         Km = Round[Transpose[Um].K.Um, 0.00000000000001];
         % // MatrixForm
         {Km // MatrixForm, ω2 // MatrixForm, Mm // MatrixForm}
         Km - ω2.Mm // MatrixForm
         Round[Det[%], .000000000000001] === 0
Out[29]= True
Out[30]= Aynisinin Mass Normalizationla
Out[32]//MatrixForm= {{1., 0, 0}, {0, 1., 0}, {0, 0, 1.}}   → M̃ = Um^T M Um → Kütle normalize ve diagonalize edilmiş modal M
Out[34]//MatrixForm= {{0.480275, 0, 0}, {0, 0.96517, 0}, {0, 0, 4.31455}}   → K̃ = Um^T K Um → Kütle normalize ve diag... modal K
Out[35]= {{{0.480275, 0, 0}, {0, 0.96517, 0}, {0, 0, 4.31455}}, {{0.480275, 0, 0}, {0, 0.96517, 0}, {0, 0, 4.31455}}, {{1., 0, 0}, {0, 1., 0}, {0, 0, 1.}}}
         K̃ = λ = [ωi^2]    λ = [ωi^2]    M̃ = I
Out[36]//MatrixForm= {{2.77556×10^-16, 0., 0.}, {0., -2.22045×10^-15, 0.}, {0., 0., -1.77636×10^-15}}   → K̃ - λM̃ = λ - λI = 0
Out[37]= True    Det|K̃ - λM̃| =? 0
In[174]:= "Modal Cozum"
          ηm = Table[Ci * Cos[Sqrt[ω2[[i, i]]] * t - ϕi], {i, 1, 3}];
          % // MatrixForm
          xm = Um.ηm;
          % // MatrixForm
          x = xm;
          1 / 2 * (D[x, t].M.D[x, t] + x.K.x)
          Simplify[%]
          1 / 2 * (ω2.ηm^2 + D[ηm, t]^2)
          Simplify[%]
Out[174]= Modal Cozum
Out[176]//MatrixForm= {Cos[0.693019 t - ϕ1] C1, Cos[0.982431 t - ϕ2] C2, Cos[2.07715 t - ϕ3] C3}   → Modal koordinatlar {ηm}
Out[178]//MatrixForm=
  -0.193239 Cos[0.693019 t - ϕ1] C1 + 0.932324 Cos[0.982431 t - ϕ2] C2 - 0.305665 Cos[2.07715 t - ϕ3]
  -4.89838 Cos[0.693019 t - ϕ1] C1 - 1.00213 Cos[0.982431 t - ϕ2] C2 + 0.0400656 Cos[2.07715 t - ϕ3]
  -0.219607 Cos[0.693019 t - ϕ1] C1 + 1.22883 Cos[0.982431 t - ϕ2] C2 + 3.88695 Cos[2.07715 t - ϕ3]
```

$x = U.\eta_m$ (Genelleştirilmiş esas koordinatlar modal koordinatlarda yazılışı)

(3)

Enerji TOP: $E_{TOP} = \frac{1}{2}(x^T K x + x'^T M x')$ Quadratik

```
Out[180]= 1/2 (0.06 (0.152192 Sin[0.693019 t - ϕ1] C1 -
     1.20724 Sin[0.982431 t - ϕ2] C2 - 8.07379 Sin[2.07715 t - ϕ3] C3)^2 +
   0.04 (3.39467 Sin[0.693019 t - ϕ1] C1 + 0.984525 Sin[0.982431 t - ϕ2] C2 -
     0.0832223 Sin[2.07715 t - ϕ3] C3)^2 +
   (0.133918 Sin[0.693019 t - ϕ1] C1 - 0.915943 Sin[0.982431 t - ϕ2] C2 +
     0.634912 Sin[2.07715 t - ϕ3] C3)^2 +
   (-4.89838 Cos[0.693019 t - ϕ1] C1 - 1.00213 Cos[0.982431 t - ϕ2] C2 +
     0.0400656 Cos[2.07715 t - ϕ3] C3)
    (-0.02 (-0.193239 Cos[0.693019 t - ϕ1] C1 + 0.932324 Cos[0.982431 t - ϕ2] C2 -
       0.305665 Cos[2.07715 t - ϕ3] C3) + 0.02 (-4.89838 Cos[0.693019 t - ϕ1] C1 -
       1.00213 Cos[0.982431 t - ϕ2] C2 + 0.0400656 Cos[2.07715 t - ϕ3] C3)) +
   (-0.193239 Cos[0.693019 t - ϕ1] C1 + 0.932324 Cos[0.982431 t - ϕ2] C2 -
     0.305665 Cos[2.07715 t - ϕ3] C3)
    (1.26 (-0.193239 Cos[0.693019 t - ϕ1] C1 + 0.932324 Cos[0.982431 t - ϕ2] C2 -
       0.305665 Cos[2.07715 t - ϕ3] C3) - 0.02 (-4.89838 Cos[0.693019 t - ϕ1] C1 -
       1.00213 Cos[0.982431 t - ϕ2] C2 + 0.0400656 Cos[2.07715 t - ϕ3] C3) -
     0.24 (-0.219607 Cos[0.693019 t - ϕ1] C1 + 1.22883 Cos[0.982431 t - ϕ2] C2 +
       3.88695 Cos[2.07715 t - ϕ3] C3)) +
   (-0.219607 Cos[0.693019 t - ϕ1] C1 + 1.22883 Cos[0.982431 t - ϕ2] C2 +
     3.88695 Cos[2.07715 t - ϕ3] C3)
    (-0.24 (-0.193239 Cos[0.693019 t - ϕ1] C1 + 0.932324 Cos[0.982431 t - ϕ2] C2 -
       0.305665 Cos[2.07715 t - ϕ3] C3) + 0.24 (-0.219607 Cos[0.693019 t - ϕ1] C1 +
       1.22883 Cos[0.982431 t - ϕ2] C2 + 3.88695 Cos[2.07715 t - ϕ3] C3)))
Out[181]= (0.240138 Cos[0.693019 t - ϕ1]^2 + 0.240138 Sin[0.693019 t - ϕ1]^2) C1^2 +
   (0.482585 Cos[0.982431 t - ϕ2]^2 + 0.482585 Sin[0.982431 t - ϕ2]^2) C2^2 +
   (-1.22645×10^-15 Cos[0.982431 t - ϕ2] Cos[2.07715 t - ϕ3] -
     1.22125×10^-15 Sin[0.982431 t - ϕ2] Sin[2.07715 t - ϕ3]) C2 C3 +
   (2.15728 Cos[2.07715 t - ϕ3]^2 + 2.15728 Sin[2.07715 t - ϕ3]^2) C3^2 +
   C1 ((-1.94289×10^-16 Cos[0.693019 t - ϕ1] Cos[0.982431 t - ϕ2] -
     4.71845×10^-16 Sin[0.693019 t - ϕ1] Sin[0.982431 t - ϕ2]) C2 +
    (1.38778×10^-16 Cos[0.693019 t - ϕ1] Cos[2.07715 t - ϕ3] -
     2.498×10^-16 Sin[0.693019 t - ϕ1] Sin[2.07715 t - ϕ3]) C3)
Out[182]= {1/2 (0.480275 Cos[0.693019 t - ϕ1]^2 C1^2 + 0.480275 Sin[0.693019 t - ϕ1]^2 C1^2),
   1/2 (0.96517 Cos[0.982431 t - ϕ2]^2 C2^2 + 0.96517 Sin[0.982431 t - ϕ2]^2 C2^2),
   1/2 (4.31455 Cos[2.07715 t - ϕ3]^2 C3^2 + 4.31455 Sin[2.07715 t - ϕ3]^2 C3^2)}
Out[183]= {0.240138 C1^2, 0.482585 C2^2, (2.15728 Cos[2.07715 t - ϕ3]^2 + 2.15728 Sin[2.07715 t - ϕ3]^2) C3^2}
```

0.2401 0 0 0 0 0 0

E_{TOP} basitleştirilmiş: $0{,}240138\,C_1^2 + 0{,}482586\,C_2^2 + 2{,}15728\,C_3^2$

$E_M = \frac{1}{2}(\omega_i^2 \eta^2 + \dot\eta^2)$

Yani $E_{TOP} = E_{Modal}$

$\Rightarrow \frac{1}{2}(x^T K x + x'^T M x') = \frac{1}{2}(\omega_i^2 \eta^2 + \dot\eta^2)$

$= \frac{1}{2}(\omega_1^2 C_1^2 + \omega_2^2 C_2^2 + \omega_3 C_3^2)$ C'ler başlangıç koşullarına bağlı

\# Peki burda Primary'nin ayrı saatlerin ayrı modal Enerjisi gözükmüyor Neden? (Çünkü bu Modal Enerji TOPLAM)

A.6 Linearization Of Nonlinear Spring K(x)=k Log(1-x(t))

Yay Tipi:Sertlesen Yay

$k \,\mathrm{Log}[1 + x[t]]$

Sistemin Toplam Kinetik Enerjisi:

$$\frac{1}{2}\sum_{i=2}^{n} m_i \,(x_i)'[t]^2 + \frac{1}{2} M_N \,(x_N)'[t]^2$$

Sistemin Toplam Potansiyel Enerjisi:

$$\sum_{i=2}^{n} k_i \,(-x_i[t] + \mathrm{Log}[1 + x_i[t] - x_N[t]]\,(1 + x_i[t] - x_N[t]) + x_N[t]) + K_N \,(-x_N[t] + \mathrm{Log}[1 + x_N[t]]\,(1 + x_N[t]))$$

Lagrange E■itli■i:

$$-\sum_{i=2}^{n} k_i \,(-x_i[t] + \mathrm{Log}[1 + x_i[t] - x_N[t]]\,(1 + x_i[t] - x_N[t]) + x_N[t]) + \frac{1}{2}\sum_{i=2}^{n} m_i \,(x_i)'[t]^2 - K_N \,(-x_N[t] + \mathrm{Log}[1 + x_N[t]]\,(1 + x_N[t])) + \frac{1}{2} M_N \,(x_N)'[t]^2$$

Hareketin Diferansiyel Deklemlerinin Euler Lagrange Denklemlerinden Cikarilmasi

$$\frac{\partial L}{\partial x_i(t)} - \frac{\partial}{\partial t}\frac{\partial L}{\partial \frac{\partial x_i(t)}{\partial t}} = 0 \qquad \frac{\partial L}{\partial x_N(t)} - \frac{\partial}{\partial t}\frac{\partial L}{\partial \frac{\partial x_N(t)}{\partial t}} = 0$$

$$-\sum_{i=2}^{n} \mathrm{Log}[1 + x_i[t] - x_N[t]]\, k_i - \frac{1}{2}\sum_{i=2}^{n} 2\, m_i \,(x_i)''[t] == 0$$

$$-\mathrm{Log}[1 + x_N[t]]\, K_N - \sum_{i=2}^{n} -\mathrm{Log}[1 + x_i[t] - x_N[t]]\, k_i - M_N \,(x_N)''[t] == 0$$

Sistemin Lineerize Edilmis Hali:

Kinetik En:

$$\frac{1}{2}\sum_{i=2}^{n} m_i \,(x_i)'[t]^2 + \frac{1}{2} M_N \,(x_N)'[t]^2$$

Pot En:

$$\sum_{i=2}^{n} \left(0.0721318\, k_i \,(x_i[t] - x_N[t]) + 0.333333\, k_i \,(x_i[t] - x_N[t])^2\right) + 0.0721318\, K_N\, x_N[t] + 0.333333\, K_N\, x_N[t]^2$$

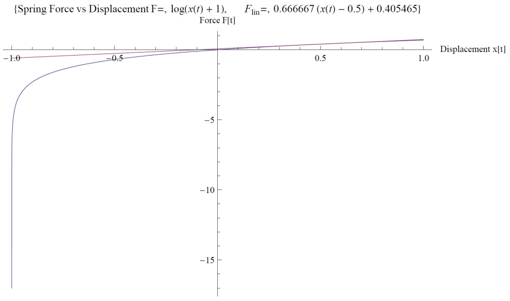
Lagrange Eq:

$$-\sum_{i=2}^{n} \left(0.0721318\, k_i \,(x_i[t] - x_N[t]) + 0.333333\, k_i \,(x_i[t] - x_N[t])^2\right) + \frac{1}{2}\sum_{i=2}^{n} m_i \,(x_i)'[t]^2 - 0.0721318\, K_N\, x_N[t] - 0.333333\, K_N\, x_N[t]^2 + \frac{1}{2} M_N \,(x_N)'[t]^2$$

$$-\sum_{i=2}^{n} (0.0721318\, k_i + 0.666667\, k_i \,(x_i[t] - x_N[t])) - \frac{1}{2}\sum_{i=2}^{n} 2\, m_i \,(x_i)''[t] == 0$$

$$-0.0721318\, K_N - \sum_{i=2}^{n} (-0.0721318\, k_i - 0.666667\, k_i \,(x_i[t] - x_N[t])) - 0.666667\, K_N\, x_N[t] - M_N \,(x_N)''[t] == 0$$

{Spring Force vs Displacement F=, $\log(x(t) + 1)$, F_{lin}=, $0.666667\,(x(t) - 0.5) + 0.405465$}



A.7 Potential Functions Leonard Jones - Morse Potential

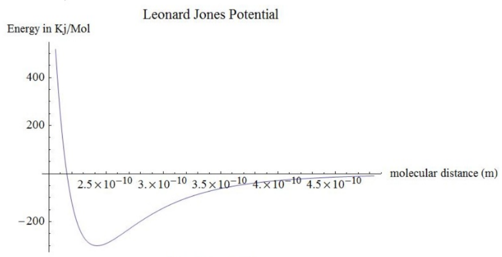
```
Avagadro=6.022142*10^23;
ze=2.42*10^-10;  (*bond distance 2.42 A in m *)
Ebond=300; (*bond Energy 300 kJ/mol *)
κ=2.55*10^10; (*decay factor in 1/angstrom*)
```

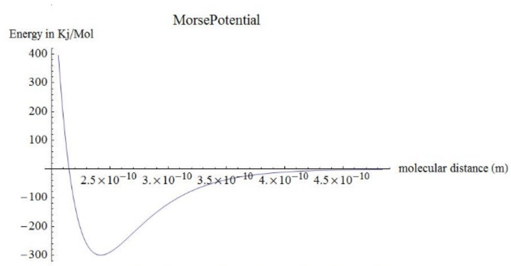
$$L = -\mathrm{Ebond}\left(2\left(\frac{ze}{z}\right)^6 - \left(\frac{ze}{z}\right)^{12}\right)$$

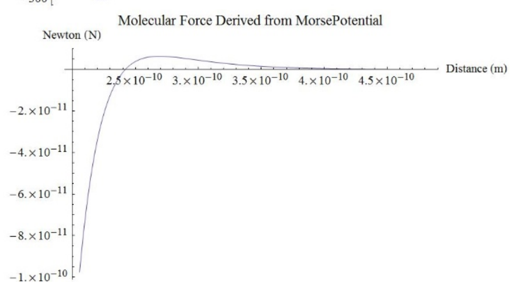
$$V = -\mathrm{Ebond}\,(2\exp(-\kappa\,(z - ze)) - \exp(-2\,\kappa\,(z - ze)))$$

$$\mathrm{Fm} = \frac{\frac{\partial V}{\partial z}}{\mathrm{Avagadro}}$$

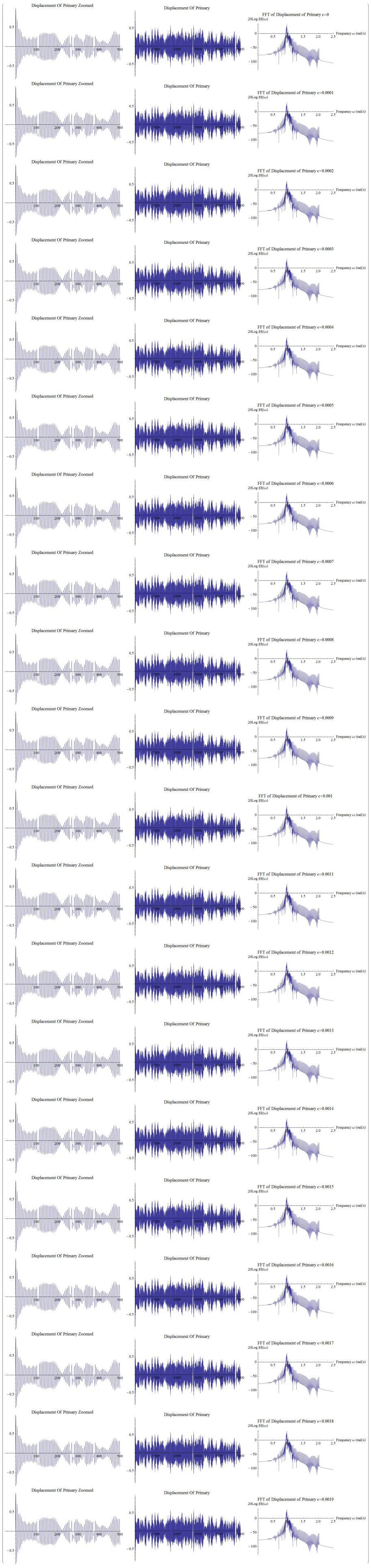
$$-4.98162\times10^{-22}\left(5.1\times10^{10}\, e^{-5.1\times10^{10}\,(-2.42\times10^{-10}+z)} - 5.1\times10^{10}\, e^{-2.55\times10^{10}\,(-2.42\times10^{-10}+z)}\right)$$







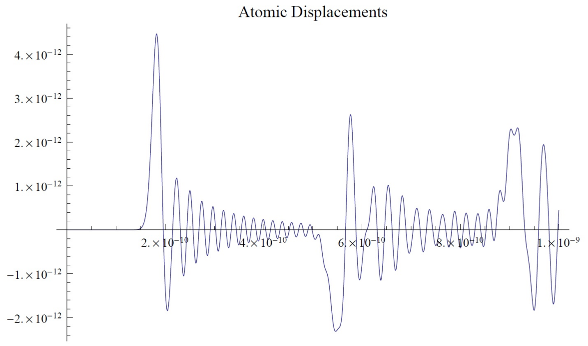
A.8 From Linear to Nonlinear - Linear Frequency Distribution with hardening spring K(x)=k (x(t) + eps x(t)^3)

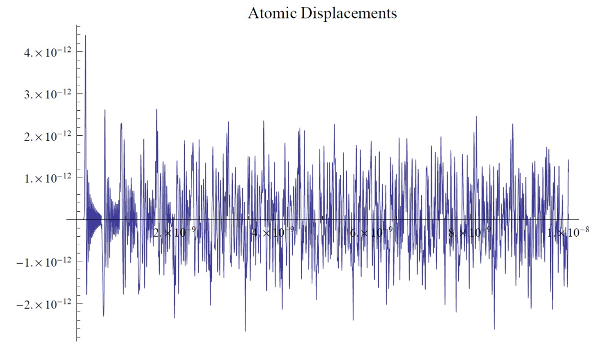


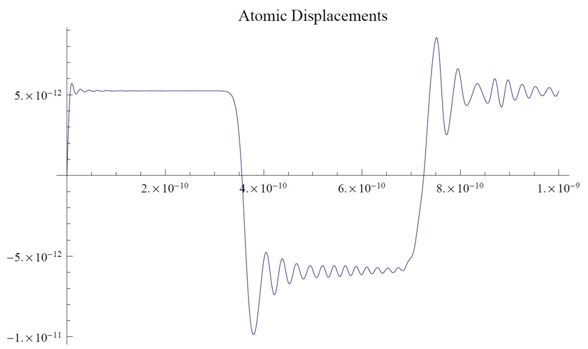

```
n = 99;
V1 = 1;
M = 1;
K = 1;
TIME = 5000;
df = 0.5;
steps = 20;

Fyay[x_, k_] = k * (x[t] + ϵ * x[t]^3);

For[i = 2, i < n + 2, ++i, mi = 0.1 / n]
For[i = 2, i < n + 2, ++i, ωi = 2 / n * i]
For[i = 2, i < n + 2, ++i, ki = ωi^2 * mi]
Clear[i];


IFk = Integrate[Fyay[x, k], x[t]];
T = 0.5 * M * x1'[t]^2 + 0.5 * Sum[mi * D[xi[t], t]^2, {i, 2, n + 1}];
V1 = IFk /. {x[t] → x1[t], k → K};
V2 = Sum[IFk /. {x[t] → xi[t] - x1[t], k → ki}, {i, 2, n + 1}];
V = V1 + V2;
L = T - V;
Eqs = Table[ D[L, xi[t]] - D[D[L, D[xi[t], t]], t] = 0 , {i, 1, n + 1} ];
AllVars = Table[xi, {i, 1, n + 1}];
InitialCon = Flatten[{Table[xi[0] = 0, {i, 1, n + 1}], Table[xi'[0] = 0, {i, 2, n + 1}], x1'[0] = 1}];

For[cnt = 1, cnt < steps + 1, cnt++,
 ϵ = 0.0001 * (cnt - 1);
 numsol = NDSolve[Flatten[Join[Eqs, InitialCon]], AllVars, {t, 0, TIME}, MaxSteps → ∞, PrecisionGoal → 12, AccuracyGoal → 12, Method → "ExplicitRungeKutta"];
 a = Abs[Fourier[Table[(x1 /. numsol[[1]])[i * df], {i, 0, TIME / df}]]];
 b = Table[{N[i / TIME * 2 π], 20 * Log[a[[i]]]}, {i, 1, TIME / df}];
 p1[cnt] = Plot[Evaluate[x1[t] /. numsol[[1]]], {t, 0, TIME}, PlotRange → {{-50, 500}, All}, ImageSize → 320, PlotLabel → "Displacement Of Primary Zoomed"];
 p2[cnt] = Plot[Evaluate[x1[t] /. numsol[[1]]], {t, 0, TIME}, PlotRange → {{-50, TIME}, All}, ImageSize → 320, PlotLabel → "Displacement Of Primary"];
 p3[cnt] = ListLinePlot[b, PlotRange → {{0, 2.5}, All} , PlotLabel → StringJoin["FFT of Displacement of Primary ϵ=", ToString[ϵ]],
   AxesLabel → {"Frequency ω (rad/s)", "20Log |H|(ω)"}, ImageSize → 320]
```

A.9 Carbon x 32 Atom Lattice Simulation ~ A Work which is inspired from Dissipation in Solids Paper

Figures : First Atom - First Atom - Last Atom - All Atoms








```
Avagadro = 6.022142 * 10^23;
ze = 2.42 * 10^-10; (*bond distance 2.42 A in m *)
Ebond = 300; (*bond Energy 300 kJ/mol *)
κ = 2.55 * 10^10; (*decay factor in 1/angstrom*)
m1 = 12 / Avagadro; (* weight of One Carbon Atom *)
IVel = 1; (* Initial Velocity of 1DOF model *)
IPos = ze; (*Initial Position of 1DOF atom *)
endtime = N[10^-8]; (*Simulation End Time*)

(*Formulas And Calculations*)
L = -Ebond * (2 * (ze / z)^6 - (ze / z)^12);
V = -Ebond * (2 * Exp[-κ * z] - Exp[-2 * κ * z]);
(*V=z^2/2;   For test Purposes*)
Va = V / Avagadro;
Fm = D[V, z] / Avagadro;

n = 32; (*lattice atoms*)
IPos = ConstantArray[0, n];
IVel = ConstantArray[0, n]; (*Initial Position of 1DOF atom *)
IVel[[n]] = 1;

Z = Table[ToExpression[StringJoin["z", ToString[i], "[t]"]], {i, 1, n}];

CarbonAtomWeight = N[12 / Avagadro];
OxygenAtomWeight = N[16 / Avagadro];

MArray = Table[CarbonAtomWeight, {i, 1, n}];
M = DiagonalMatrix[MArray];

VPotTemp = Total[Table[Va /. z → (Z[[i]] - Z[[i + 1]]), {i, 1, n - 1}]];
VPot = (Va /. z → Z[[1]]) + VPotTemp;


TKin = Sum[0.5 * M[[i, i]] * D[Z[[i]], t]^2, {i, 1, n}];
Lagrange = TKin - VPot ;

temp1 = Table[D[Lagrange, D[Z[[i]], t], t] - D[Lagrange, Z[[i]] ] == 0, {i, 1, n}];
temp2 =
  Table[{(Z[[i]] /. t → 0) == IPos[[i]], (D[Z[[i]], t] /. t → 0) == IVel[[i]]}, {i, 1, n}];

Eqs = Flatten[{temp1, temp2}];


solMDOF =
  NDSolve[Eqs, Z, {t, 0, endtime}, MaxSteps → ∞, PrecisionGoal → 13, AccuracyGoal → 13];
Plot[Evaluate[Z[[1]] /. solMDOF], {t, 0, endtime}, PlotRange → All,
  PlotLabel → "Atomic Displacements", ImageSize → 420]
 Plot[Evaluate[Z[[1]] /. solMDOF], {t, 0, endtime / 10}, PlotRange → All,
  PlotLabel → "Atomic Displacements", ImageSize → 420]
Plot[Evaluate[Z[[n]] /. solMDOF], {t, 0, endtime / 10}, PlotRange → All,
 PlotLabel → "Atomic Displacements", ImageSize → 420]
Plot[Evaluate[Z /. solMDOF], {t, 0, endtime / 10}, PlotRange → All,
 PlotLabel → "Atomic Displacements", ImageSize → 420]
```