In[7]:=
```
SetDirectory[NotebookDirectory[]]
```

Out[7]=
```
D:\VS_workspace\CPlusPlus\SOHR\projects\catalytic_cycle\theory\wall_S_chattering_problem
```

$A \underset{k2}{\overset{k1}{\rightleftharpoons}} B \xrightarrow{k3} C$ problem

Solve differential equation like

$$\frac{d[A]}{dt} = -k1[A] + k2[B]$$

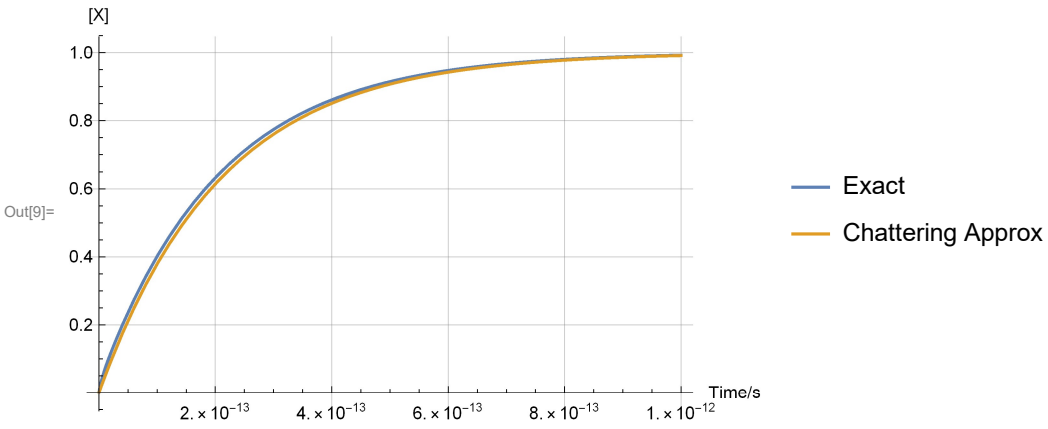
$$\frac{d[B]}{dt} = k1[A] - k2[B] - k3[B]$$

$$\frac{d[C]}{dt} = k3[B]$$

In[8]:=
```
(*left hand side of equation in terms of k1, k2,
k3 and t, Here we calculate the concentration of C*)
Clear[ExactSolnC]; ExactSolnC[k1_, k2_, t_, k3_] :=
 Module[{soln, output, x1, x2, x3},
  soln = DSolve[{x1'[t] == -k1 * x1[t] + k2 * x2[t],
     x2'[t] == k1 * x1[t] - (k2 + k3) * x2[t], x3'[t] == k3 * x2[t],
     x1[0] == 0, x2[0] == 1.0, x3[0] == 0}, {x1[t], x2[t], x3[t]}, t];
  output = Simplify[x3[t] /. soln[[1, 3]], Assumptions → {k1 > 0, k2 > 0, k3 > 0, t > 0}];
  Return[output];]
```

In[9]:=
```
Value1 = {k1 → 10^14, k2 → 10^14, k3 → 10^13};
Plot[{ExactSolnC[k1, k2, t, k3] /. Value1 // Evaluate, 1 - e^-(k3*k1/(k3+k1+k2))*t /. Value1},
 {t, 0, 10^-12}, PlotLegends → {"Exact", "Chattering Approx"},
 GridLines → Automatic, AxesLabel → {"Time/s", "[X]"}]
```

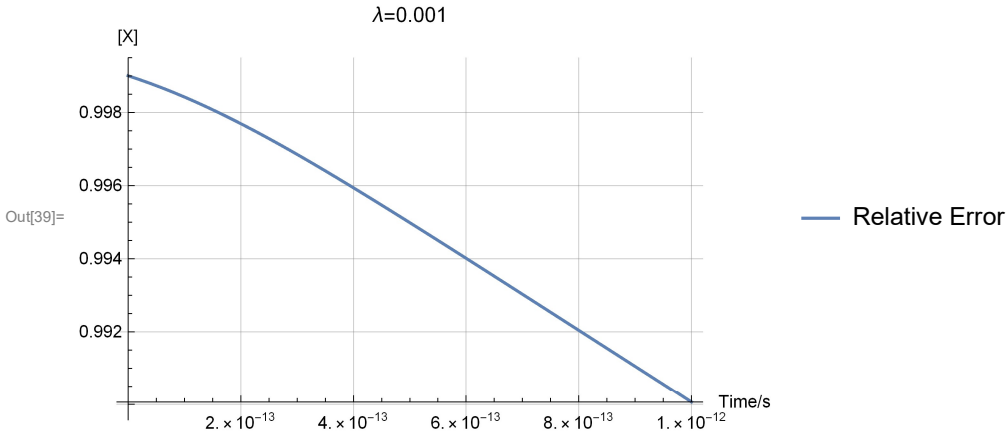
Out[9]=



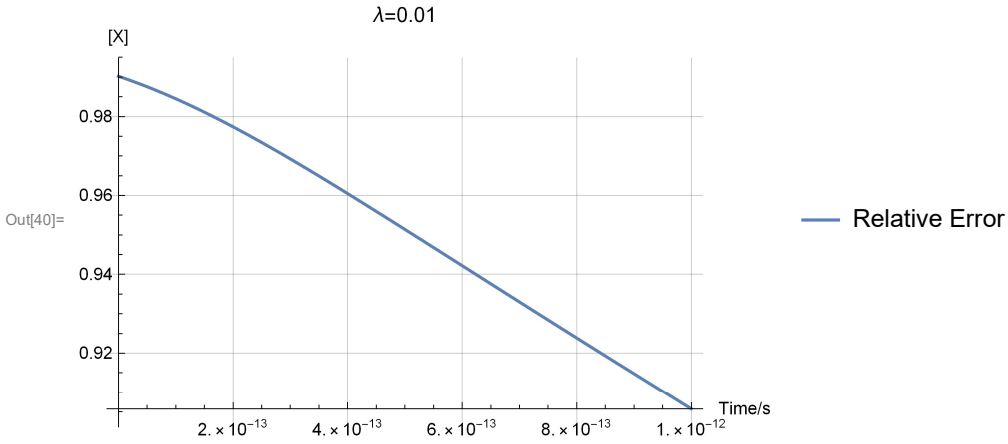
In[30]:=
```
Clear[PLOTERROR]; PLOTERROR[kbasein_, endTime_, λin_] := Module[
  {k1, k2, k3, λ, t, Value1, kbase},
  Value1 = {k1 → λ * kbase, k2 → λ * kbase, k3 → kbase} /. {kbase → kbasein, λ → λin};
  Plot[((ExactSolnC[k1, k2, t, k3] - (1 - e^-(k3*k1/(k3+k1+k2))*t)) / ExactSolnC[k1, k2, t, k3] /.
     Value1 // Evaluate, {t, 0, endTime}, PlotLegends → {"Relative Error"}, GridLines →
   Automatic, AxesLabel → {"Time/s", "[X]"}, PlotLabel → "λ=" <> ToString[N[λin]]]];
```

In[39]:=
```
PLOTERROR[10^13, 10^-12, 10^-3]
PLOTERROR[10^13, 10^-12, 10^-2]
PLOTERROR[10^13, 10^-12, 10^-1]
PLOTERROR[10^13, 10^-12, 10^-0]
PLOTERROR[10^13, 10^-12, 10^1]
PLOTERROR[10^13, 10^-12, 10^2]
PLOTERROR[10^13, 10^-12, 10^3]
```

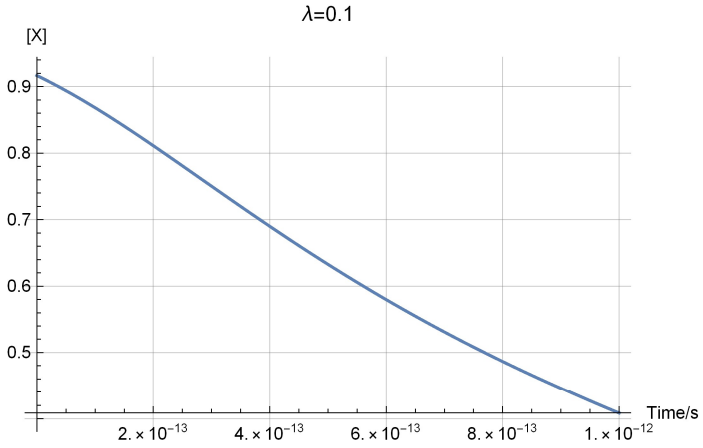
Out[39]=



Out[40]=

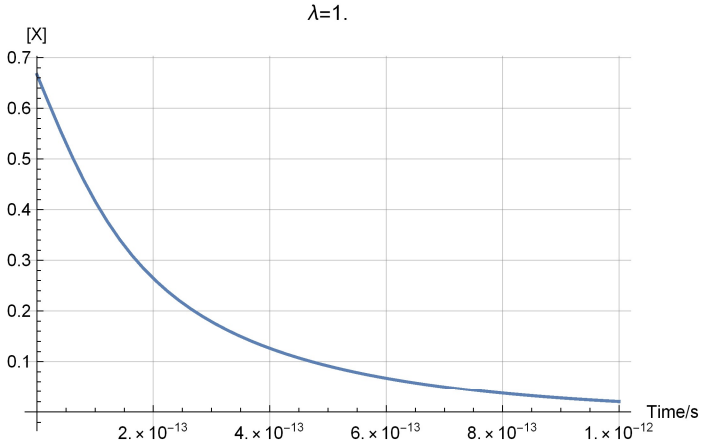


Out[41]=



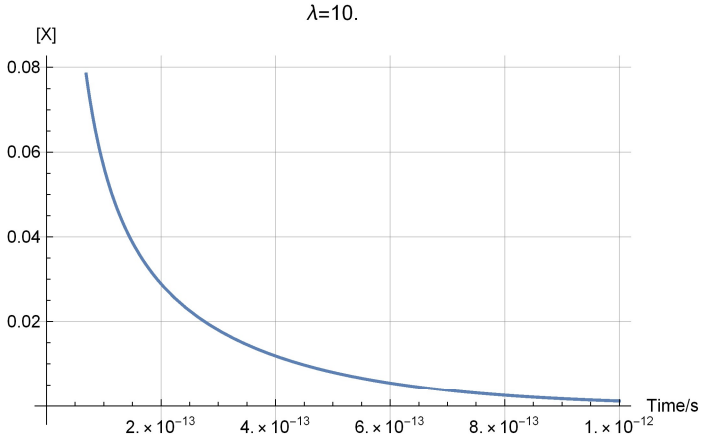
Relative Error

Out[42]=



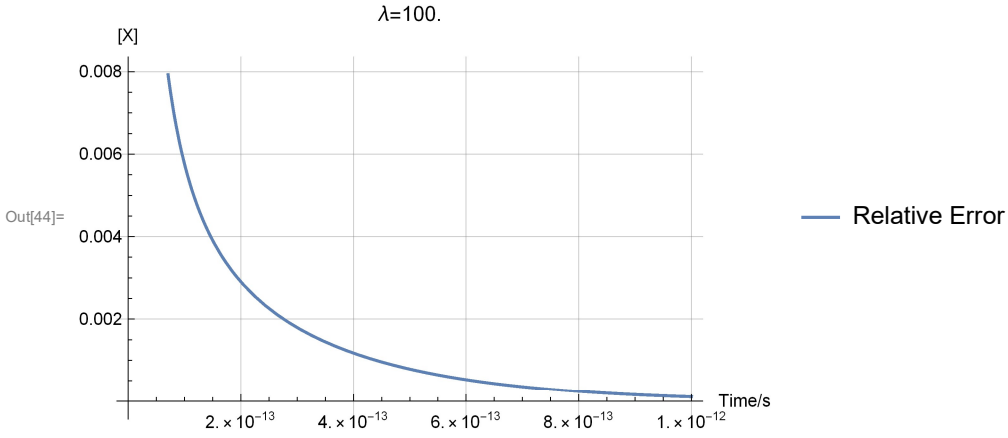
Relative Error

Out[43]=

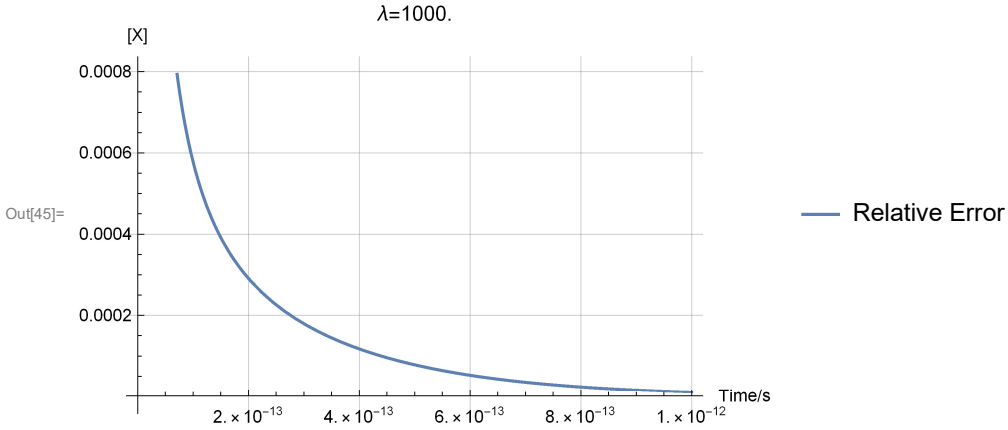


Relative Error

Out[44]=


λ=100.
[X]
0.008
0.006
0.004
0.002
2. × 10^-13
4. × 10^-13
6. × 10^-13
8. × 10^-13
1. × 10^-12
Time/s
Relative Error

Out[45]=


λ=1000.
[X]
0.0008
0.0006
0.0004
0.0002
2. × 10^-13
4. × 10^-13
6. × 10^-13
8. × 10^-13
1. × 10^-12
Time/s
Relative Error