(*
Example of Using the Nudged Elastic–Band Method to Find a Minimum–Energy Path
*)

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d1 = 0.0;
d2 = 1.0;
PES[x_, y_] := Cos[2 π x] (1 + d1 y) + d2/2 2 π y^2;
XGrad[x_, y_] := -2 π Sin[2 π x] (1 + d1 y);
YGrad[x_, y_] := 2 d2 π y + d1 Cos[2 π x];
TOTGrad[x_, y_] := XGrad[x, y] + YGrad[x, y];
(*
 Number of Images to Include
 *)
Nim = 5;
Ninc = 1.0 / (Nim - 1);
(*
 Set Maximum Number of Iterations and Spring Constant
 *)
tmax = 200000.0;
ks = 5.0;
(*
 Find Neighboring Minima
 *)
Print["Minima of the PES"]
x1 = -0.5;
a = FindRoot[TOTGrad[x1, y] == 0, {y, 0.0}];
y1 = Evaluate[y /. a];
xN = 0.5;
b = FindRoot[TOTGrad[xN, y] == 0, {y, 0.0}];
yN = Evaluate[y /. b];
Print[x1, " ", y1]
Print[xN, " ", yN]
(*
 Solve for the MEP - First, Define the Equations
 *)
eqns = Join[{x[2]'[t] == (2 π Sin[2 π x[2][t]] (1 + d1 y[2][t]))
    (1 - ((x[3][t] - x1) / Sqrt[(x[3][t] - x1)^2 + (y[3][t] - y1)^2])^2) +
   ks (Sqrt[(x[3][t] - x[2][t])^2 + (y[3][t] - y[2][t])^2] -
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$$\sqrt{(x[2][t]-x1)^2+(y[2][t]-y1)^2}\Bigg)$$

$$\left(\frac{x[3][t]-x1}{\sqrt{(x[3][t]-x1)^2+(y[3][t]-y1)^2}}\right)\Bigg\},$$

$$\{y[2]'[t] == -(2\,d2\,\pi\,y[2][t]+d1\,\mathrm{Cos}[2\,\pi\,x[2][t]])$$

$$\left(1-\left(\frac{y[3][t]-y1}{\sqrt{(x[3][t]-x1)^2+(y[3][t]-y1)^2}}\right)^2\right)+$$

$$ks\Bigg(\sqrt{(x[3][t]-x[2][t])^2+(y[3][t]-y[2][t])^2}-$$

$$\sqrt{(x[2][t]-x1)^2+(y[2][t]-y1)^2}\Bigg)$$

$$\left(\frac{y[3][t]-y1}{\sqrt{(x[3][t]-x1)^2+(y[3][t]-y1)^2}}\right)\Bigg\},\ \mathrm{Table}\Big[$$

$$x[i]'[t] == (2\,\pi\,\mathrm{Sin}[2\,\pi\,x[i][t]]\,(1+d1\,y[i][t]))\Bigg(1-$$

$$\left(\frac{x[i+1][t]-x[i-1][t]}{\sqrt{(x[i+1][t]-x[i-1][t])^2+(y[i+1][t]-y[i-1][t])^2}}\right)^2\Bigg)$$

$$+$$

$$ks$$

$$\Bigg(\sqrt{(x[i+1][t]-x[i][t])^2+(y[i+1][t]-y[i][t])^2}-$$

$$\sqrt{(x[i][t]-x[i-1][t])^2+(y[i][t]-y[i-1][t])^2}\Bigg)$$

$$\left(\frac{x[i+1][t]-x[i-1][t]}{\sqrt{(x[i+1][t]-x[i-1][t])^2+(y[i+1][t]-y[i-1][t])^2}}\right)$$

$$,\ \{i,\ 3,\ (Nim-2)\}\Big],$$

$$\text{Table}\Bigg[y[i]'[t] == -(2\,d2\,\pi\,y[i][t] + d1\,\text{Cos}[2\,\pi\,x[i][t]])\left(1 - \left(\frac{y[i+1][t] - y[i-1][t]}{\sqrt{(x[i+1][t] - x[i-1][t])^2 + (y[i+1][t] - y[i-1][t])^2}}\right)^2\right) +$$

$$ks\left(\sqrt{(x[i+1][t] - x[i][t])^2 + (y[i+1][t] - y[i][t])^2} - \sqrt{(x[i][t] - x[i-1][t])^2 + (y[i][t] - y[i-1][t])^2}\right)$$

$$\left(\frac{y[i+1][t] - y[i-1][t]}{\sqrt{(x[i+1][t] - x[i-1][t])^2 + (y[i+1][t] - y[i-1][t])^2}}\right), \{i, 3, (Nim-2)\}\Bigg], \Big\{x[(Nim-1)]'[t] ==$$

$$(2\,\pi\,\text{Sin}[2\,\pi\,x[(Nim-1)][t]]\,(1 + d1\,y[(Nim-1)][t]))$$

$$\left(1 - \left(\frac{xN - x[(Nim-2)][t]}{\sqrt{(xN - x[(Nim-2)][t])^2 + (yN - y[(Nim-2)][t])^2}}\right)^2\right) +$$

$$ks\left(\sqrt{(xN - x[(Nim-1)][t])^2 + (yN - y[(Nim-1)][t])^2} - \sqrt{\left((x[(Nim-1)][t] - x[(Nim-2)][t])^2 + (y[(Nim-1)][t] - y[(Nim-2)][t])^2\right)}\right)$$

$$\left(\frac{xN - x[(Nim-2)][t]}{\sqrt{(xN - x[(Nim-2)][t])^2 + (yN - y[(Nim-2)][t])^2}}\right)\Big\},$$

$$\{y[(Nim-1)]'[t] == -(2\,d2\,\pi\,y[(Nim-1)][t] + d1\,\text{Cos}[2\,\pi\,x[(Nim-1)][t]])$$

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(1 - ((yN - y[(Nim - 2)][t]) / Sqrt[(xN - x[(Nim - 2)][t])^2 + (yN - y[(Nim - 2)][t])^2])^2) +
  ks (Sqrt[(xN - x[(Nim - 1)][t])^2 + (yN - y[(Nim - 1)][t])^2] -
     Sqrt[((x[(Nim - 1)][t] - x[(Nim - 2)][t])^2 +
        (y[(Nim - 1)][t] - y[(Nim - 2)][t])^2)])
   ((yN - y[(Nim - 2)][t]) / Sqrt[(xN - x[(Nim - 2)][t])^2 + (yN - y[(Nim - 2)][t])^2])}];
(*
 Initial Condition
 *)
eqns = Join[eqns, Table[x[i][0] == (x1 - Ninc) + Ninc i, {i, 2, (Nim - 1)}],
   Table[y[i][0] == 0.0, {i, 2, (Nim - 1)}]];
(*
 Generate a Table for the Remaining Required Input.
 *)
seqns =
  Join[Table[x[i], {i, 2, (Nim - 1)}], Table[y[i], {i, 2, (Nim - 1)}]]
(*
 Solve Equations, Store the solution in sol
 *)
sol = NDSolve[eqns, seqns, {t, tmax}];
(*
 Format MEP in a Suitable Plotting Form
 *)
xpath = Flatten[
   Append[{x1}, Flatten[Table[{Evaluate[x[i][tmax] /. sol]}, {i, 2, (Nim - 1)}]]]];
xpath = Flatten[Append[xpath, {xN}]];
ypath = Flatten[
   Append[{y1}, Flatten[Table[{Evaluate[y[i][tmax] /. sol]}, {i, 2, (Nim - 1)}]]]];
ypath = Flatten[Append[ypath, {yN}]];
path = Join[xpath, ypath];
path = Partition[path, Dimensions[xpath]];
Print["Coordinates of MEP"]
path = Transpose[path]
$TextStyle = {FontSize → 16};
(*
 Plot the PES and MEP
```

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 *)
$TextStyle = {FontSize → 16};
Print["Potential-Energy Surface"]
Plot3D[PES[x, y], {x, -1, 1}, {y, -1, 1},
  PlotPoints → 20 , AxesLabel → {"x", "y", "V(x,y)"}];
p1 = Show[ContourGraphics[%], Contours → 20,
   ColorFunction → Hue, FrameLabel → {"x", "y"}];
p2 = ListPlot[path, Prolog -> AbsolutePointSize[5],
   Frame -> True, PlotJoined -> True];
p3 = ListPlot[path, Prolog -> AbsolutePointSize[5],
   Frame -> True];
Show[p1, p2, p3, Prolog -> AbsolutePointSize[5]]
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Minima of the PES

-0.5 0.

0.5 0.

Coordinates of MEP

{{-0.5, 0.}, {-0.25, 0.}, {0., 0.}, {0.25, 0.}, {0.5, 0.}}

Potential-Energy Surface
```

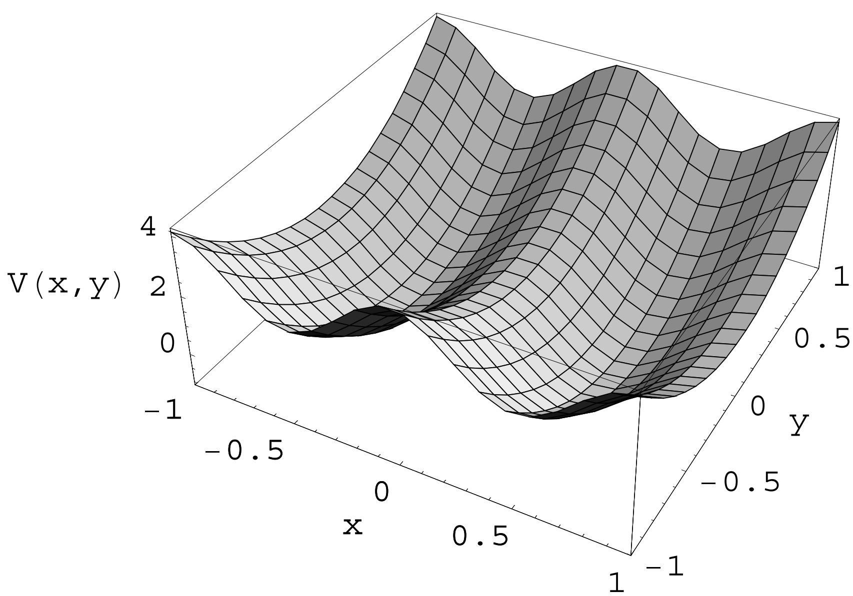

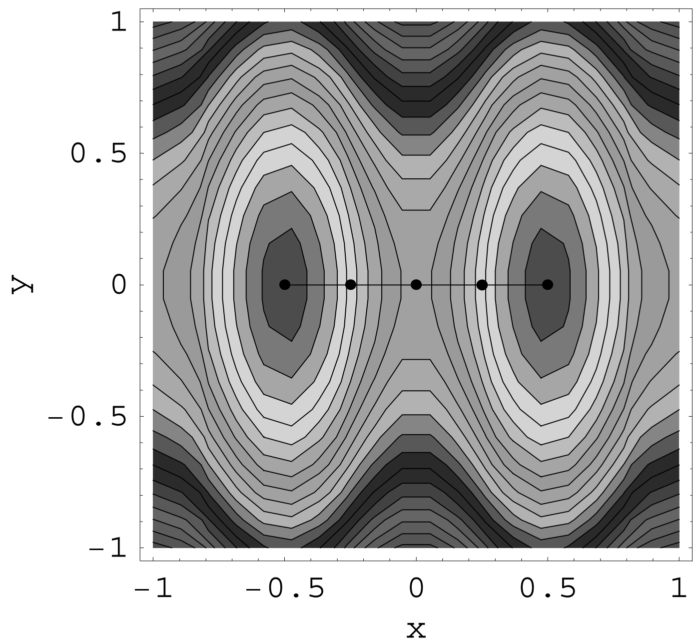

- Graphics -