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(*
MATHEMATICA DEMO OF PARALLEL TEMPERING
MONTE CARLO – PART 2: PARALLEL TEMPERING
*)
<< Graphics`MultipleListPlot`
<< Graphics`Legend`
$TextStyle = {FontSize -> 14}
(*
INITIALIZE ARRAYS,
TEMPERATURES, AND MAXIMUM NUMBER OF MCS
*)
MaxTrials = 300000;
hist = Table[0, {i, 100}, {j, 3}];
tot1 = Table[0, {i, 100}, {j, 2}];
tot2 = Table[0, {i, 100}, {j, 2}];
tot3 = Table[0, {i, 100}, {j, 2}];
pot = Table[0, {i, 100}, {j, 2}];
displ = Table[0, {i, MaxTrials}];
a = Table[0, {i, 3}];
U = Table[0, {i, 3}];
kT = Table[0, {i, 3}];
kT[[1]] = 0.05;
kT[[2]] = 0.5;
kT[[3]] = 5.0;
(*
INITIALIZE THE PARTICLE POSITIONS AND ENERGIES
*)
Do[{
  a[[ens]] = Random[Real, {-1.5, -1.0}];
  U[[ens]] = 1 + Sin[2  $\pi$  a[[ens]]];
  If[-1.25  $\leq$  a[[ens]] && a[[ens]]  $\leq$  -0.25,
    {U[[ens]] = 2 U[[ens]]},
    {If[-0.25  $\leq$  a[[ens]] && a[[ens]]  $\leq$  0.75,
      {U[[ens]] = 3 U[[ens]]},
      {If[0.75  $\leq$  a[[ens]] && a[[ens]]  $\leq$  1.75,
        {U[[ens]] = 4 U[[ens]]},
        {If[1.75  $\leq$  a[[ens]] && a[[ens]]  $\leq$  2.0,
          U[[ens]] = 5 U[[ens]]}}}}}], {ens, 1, 3}];
displ[[1]] = a[[1]];
(*
THE MONTE CARLO LOOP
*)
Do[{
  (*
    Randomly Select an Ensemble and a Switching Probability
    *)

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ens = Random[Integer, {1, 3}];
swch = Random[];
If[swch ≤ 0.9,
(*
Metropolis Trial Within Selected System
*)
{triala = Random[Real, {-0.1, 0.1}];
 anew = a[[ens]] + triala;
(*
Calculate the Energy
*)
If[-2 ≤ anew && anew ≤ 2,
 {Unew = 1 + Sin[2 π anew];
  If[-1.25 ≤ anew && anew ≤ -0.25,
   {Unew = 2 Unew},
   {If[-0.25 ≤ anew && anew ≤ 0.75,
    {Unew = 3 Unew},
    {If[0.75 ≤ anew && anew ≤ 1.75,
     {Unew = 4 Unew},
     {If[1.75 ≤ anew && anew ≤ 2.0,
      Unew = 5 Unew}}}}]}],
 {Unew = 5 106}}];
If[Unew ≤ U[[ens]],
 {a[[ens]] = anew;
  U[[ens]] = Unew},
 {boltz = Exp[-(Unew - U[[ens]]) / kT[[ens]]];
  p = Random[];
  If[p < boltz,
   {a[[ens]] = anew;
    U[[ens]] = Unew}}];
(*
Update Displacement Histogram
*)
ihist = IntegerPart[1 + (100.0 (2.0 + a[[ens]]) / 4.0)];
hist[[ihist, ens]] = hist[[ihist, ens]] + 1,
(*
Swap of Two Different Ensembles
*)
{ens1 = Random[Integer, {1, 3}];
 boltz = Exp[-(U[[ens1]] - U[[ens]]) (1 / kT[[ens]] - 1 / kT[[ens1]])]
 If[boltz ≥ 1.0,
  {temp = a[[ens]];
   a[[ens]] = a[[ens1]];
   a[[ens1]] = temp;
   temp = U[[ens]];
   U[[ens]] = U[[ens1]];
   U[[ens1]] = temp},
 {p = Random[];

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If[p < boltz,
  {temp = a[[ens]];
   a[[ens]] = a[[ens1]];
   a[[ens1]] = temp;
   temp = U[[ens]];
   U[[ens]] = U[[ens1]];
   U[[ens1]] = temp}}];

(*
Update Displacement Histogram
*)
ihist = IntegerPart[1 + (100.0 (2.0 + a[[ens]]) / 4.0)];
hist[[ihist, ens]] = hist[[ihist, ens]] + 1;
ihist = IntegerPart[1 + (100.0 (2.0 + a[[ens1]]) / 4.0)];
hist[[ihist, ens1]] = hist[[ihist, ens1]] + 1;
displ[[trials]] = a[[1]];
{trials, 1, MaxTrials}];

(*
Prepare Displacement Histograms and Potential for Plotting
*)
hist = hist / (3.0 MaxTrials);
Do[
  {tot1[[i, 1]] = 4.0 i / 100.0 - 2.0;
   tot1[[i, 2]] = hist[[i, 1]];
   tot2[[i, 1]] = tot1[[i, 1]];
   tot2[[i, 2]] = hist[[i, 2]];
   tot3[[i, 1]] = tot1[[i, 1]];
   tot3[[i, 2]] = hist[[i, 3]];
   pot[[i, 1]] = tot1[[i, 1]];
   pot[[i, 2]] = 1 + Sin[2  $\pi$  pot[[i, 1]]];
   If[-1.25  $\leq$  pot[[i, 1]] && pot[[i, 1]]  $\leq$  -0.25,
     {pot[[i, 2]] = 2 pot[[i, 2]]},
     {If[-0.25  $\leq$  pot[[i, 1]] && pot[[i, 1]]  $\leq$  0.75,
       {pot[[i, 2]] = 3 pot[[i, 2]]},
       {If[0.75  $\leq$  pot[[i, 1]] && pot[[i, 1]]  $\leq$  1.75,
         {pot[[i, 2]] = 4 pot[[i, 2]]},
         {If[1.75  $\leq$  pot[[i, 1]] && pot[[i, 1]]  $\leq$  2.0,
           pot[[i, 2]] = 5 pot[[i, 2]]}}}}},
   {i, 1, 100}];
Print["Potential"]
ListPlot[pot, PlotJoined  $\rightarrow$  True,
  PlotRange  $\rightarrow$  All, Frame  $\rightarrow$  True, FrameLabel  $\rightarrow$  {"x", "U(x)"}];
Print["Displacement Histograms"]
(*ListPlot[tot1, PlotJoined  $\rightarrow$  True,
  PlotRange  $\rightarrow$  All, Frame  $\rightarrow$  True, FrameLabel  $\rightarrow$  {"x", "P(x)"}];
ListPlot[tot2, PlotJoined  $\rightarrow$  True, PlotRange  $\rightarrow$  All,
  Frame  $\rightarrow$  True, FrameLabel  $\rightarrow$  {"x", "P(x)"}];
ListPlot[tot3, PlotJoined  $\rightarrow$  True, PlotRange  $\rightarrow$  All,
  Frame  $\rightarrow$  True, FrameLabel  $\rightarrow$  {"x", "P(x)"}]; *)
MultipleListPlot[tot1, tot2, tot3, PlotJoined  $\rightarrow$  True,

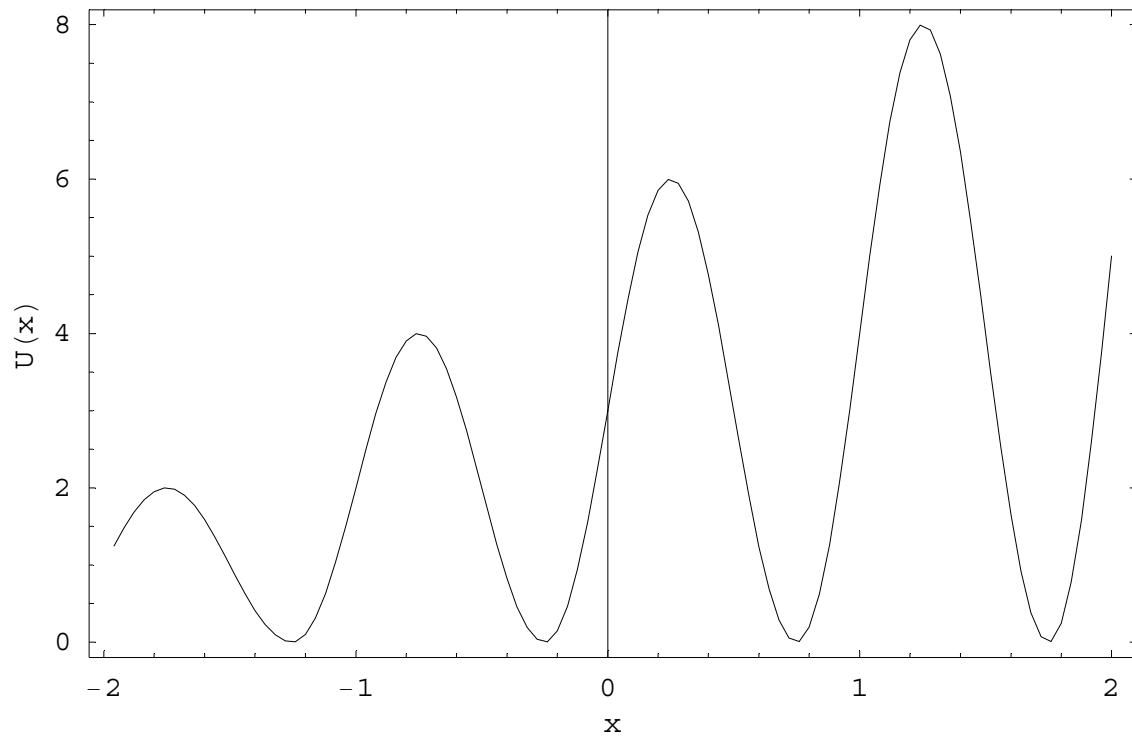
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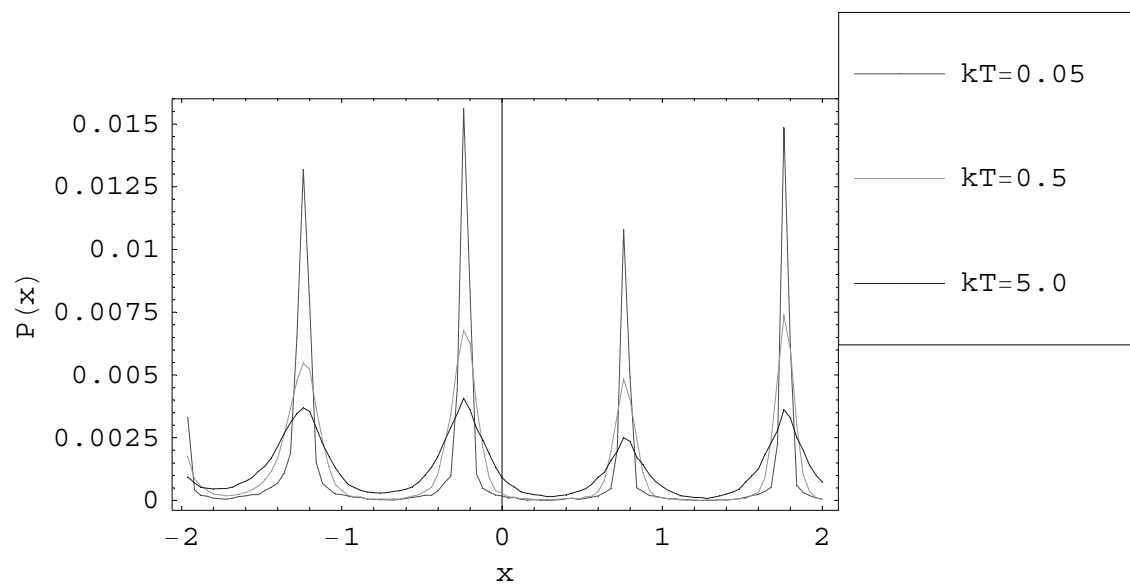
SymbolShape → {PlotSymbol[Box, 0.1, Filled → True],
  PlotSymbol[Box, 0.1, Filled → True], PlotSymbol[Box, 0.1, Filled → True]},
SymbolStyle → {RGBColor[1, 0, 0], RGBColor[0, 1, 0], RGBColor[0, 0, 1]},
PlotStyle → {RGBColor[1, 0, 0], RGBColor[0, 1, 0], RGBColor[0, 0, 1]},
PlotLegend → {"kT=0.05", "kT=0.5", "kT=5.0"}, LegendPosition → {1, 0},
LegendShadow → {0, 0}, PlotRange → All, Frame → True, FrameLabel → {"x", "P(x)"};
Print["Displacement of Particle at kT=0.05"]
ListPlot[displ, PlotJoined → True,
  PlotRange → All, Frame → True, FrameLabel → {"Trials", "x"}];
{FontSize → 14}

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Potential



Displacement Histograms

Displacement of Particle at $kT=0.05$ 