
```

In[51]:= (*

$$\text{MATHEMATICA DEMO OF KINETIC MONTE CARLO}$$


$$\text{FOR LANGMUIR ADSORPTION-DESORPTION}$$

*)

<< Graphics`Legend`
<< Graphics`MultipleListPlot`
$TextStyle = {FontSize -> 14};
(*

$$\text{INITIALIZE LATTICE DIMENSIONS}$$


$$\text{AND MAXIMUM NUMBER OF MCS}$$

*)

L = 20;
LTOT = L^2;
MCS = 100;
MaxTrials = MCS LTOT + 1;
Rads = 0.5;
Rdes = 0.5;
(*

$$\text{INITIALIZE THE LATTICE}$$

*)

NO = 0;
lattice = Table[0, {i, L}, {j, L}];
θ = Table[0, {i, MaxTrials}];
τ = Table[0, {i, MaxTrials}];
tot = Table[0, {i, MaxTrials}, {j, 2}];
sol = Table[0, {i, MaxTrials}, {j, 2}];
θ[[1]] = 0.0;
τ[[1]] = 0.0;
(*

$$\text{THE MONTE CARLO LOOP}$$

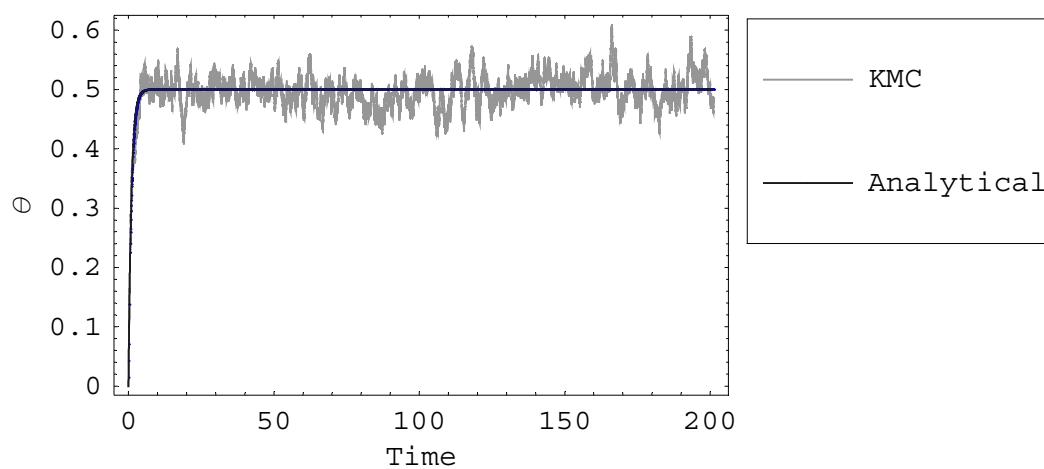
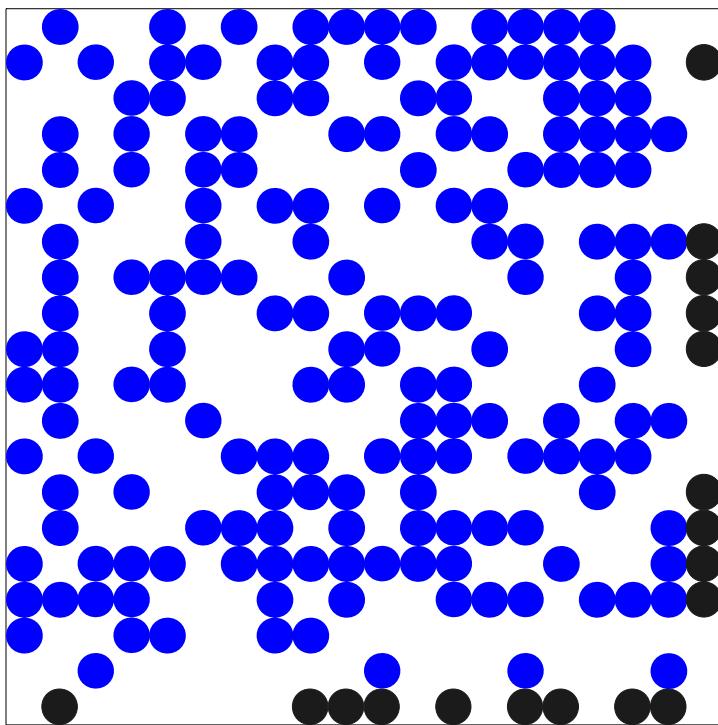
*)

Do[
  pads = 
$$\frac{(LTOT - NO) Rads}{(LTOT - NO) Rads + NO Rdes}$$
;
  notdone = True;
  p = Random[];
  If[p ≤ pads,
    {While[notdone,
      {a = Random[Integer, {1, L}];
       b = Random[Integer, {1, L}];
       If[lattice[[a, b]] == 0,
         {lattice[[a, b]] = 1;
          NO = NO + 1;
          notdone = False}]]};},
    {While[notdone,
      {a = Random[Integer, {1, L}];
```

```

b = Random[Integer, {1, L}];
If[lattice[[a, b]] == 1,
{lattice[[a, b]] = 0;
NO = NO - 1;
notdone = False}]]];
θ[[k]] = 1.0 NO / LTOT;
Rtot = NO Rdes + (LTOT - NO) Rads;
rr = Random[];
τ[[k]] = τ[[k - 1]] - Log[rr] / Rtot}, {k, 2, MaxTrials}];
Do[
{tot[[i, 1]] = τ[[i]];
tot[[i, 2]] = θ[[i]];
sol[[i, 1]] = τ[[i]];
sol[[i, 2]] =  $\left( \frac{\text{Rads}}{\text{Rads} + \text{Rdes}} \right) (1 - \text{Exp}[-(\text{Rads} + \text{Rdes}) \tau[[i]]])$ ,
{i, 1, MaxTrials}];
Clist = Table[0, {i, NO}, {j, 2}];
NA = 0;
Do[
{If[lattice[[i, j]] == 1,
{NA = NA + 1;
Clist[[NA, 1]] = i;
Clist[[NA, 2]] = j}
]], {i, L}, {j, L}];
Print["Final Lattice Configuration"];
ListPlot[Clist, Axes → False, AspectRatio → Automatic,
PlotRange → {{0.5, L + 0.5}, {0.5, L + 0.5}},
PlotStyle → {PointSize[0.05], RGBColor[0, 0, 1]}, Frame → True, FrameTicks → None];
MultipleListPlot[tot, sol, PlotJoined → {True, True}, SymbolShape →
{PlotSymbol[Box, 0.1, Filled → True], PlotSymbol[Box, 0.1, Filled → True]},
SymbolStyle → {RGBColor[0, 1, 0], RGBColor[0, 0, 1]},
PlotStyle → {{RGBColor[0, 1, 0], AbsoluteThickness[1.0]},
{RGBColor[0, 0, 1], AbsoluteThickness[1.0]}}, PlotLegend → {"KMC", "Analytical"},
LegendPosition → {1, 0}, LegendShadow → {0, 0}, PlotRange → All,
AxesOrigin → 0, Frame → True, FrameLabel → {"Time", "θ"}];
Final Lattice Configuration

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In [75]:=