Mathematica 4.2 - [energygap.nb]

File   Edit   Cell   Format   Input   Kernel   Find   Window   Help

Evaluation	▶	Evaluate Cells
Interrupt Evaluation... Alt+,		Evaluate in Place
Abort Evaluation Alt+.		Evaluate Next Input
		Evaluate in Subsession
Start Kernel ▶		
Quit Kernel ▶		Evaluate Notebook
Default Kernel ▶		Evaluate Initialization
Notebook's Kernel ▶		
Kernel Configuration Options...		Enter Subsession
		Exit Subsession
✔ Show In/Out Names		
Delete All Output		Remove from Evaluation

energygap.nb

```
(* The gap function, E

gapfuncfile = ReadList

gapfunc = Table[gapfun

ListPlot[gapfunc, PlotJ
   PlotStyle → { RGBColor
```

```
(*
 Now read the sample output from a longer (10 ps) simulation
  You are given a larger data file to read for this.
 *)

EpsilonOfTfile = ReadList["dataLONG.dat", {Number, Number}];
EpsilonOfT = Table[EpsilonOfTfile[[k]][[2]], {k, Length[EpsilonOfTfile]}];
noframes = Length[EpsilonOfTfile];

ListPlot[EpsilonOfT, PlotJoined → True, PlotRange → All, Axes → False, Frame → True,
   PlotStyle → { RGBColor[0.2, 0., 0.5]}];

<< Graphics`Graphics`

<< Statistics`DescriptiveStatistics`

Histogram[EpsilonOfT, Frame → True];



(*  mean and variance of epsilon (t) *)

meanEps = Sum[EpsilonOfT[[k]], {k, noframes}] / noframes

varianceEps = Sqrt[ (Sum[ (EpsilonOfT[[k]] - meanEps) ^2, {k, noframes}]) / noframes]
```