

W.Quapp and J.M.Bofill

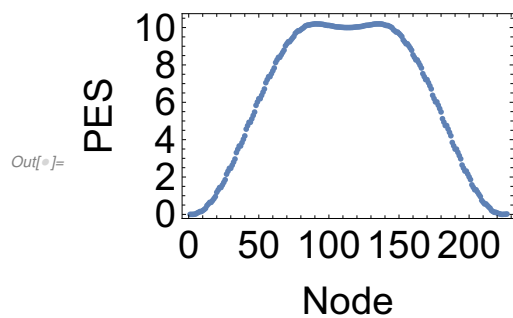
Sliding Paths for Series of Frenkel – Kontorova Models–
A contribution to the concept of 1 D – superlubricity

Supplementary Material 6

MF 1 N = 5, ... 20

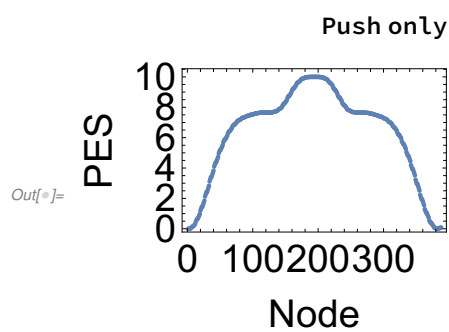
NoMisfit = 1

N = 5 profile energy5DdirPP



stat SP1 node115 energy = 9.9984369412 detHess 1.00
3.1374591163 × 9.4289119537 × 15.7162308100
21.9952822184 × 28.2701999953
ok there is only one SP1 ; peaks are TPs !

gMin node226 energy = 0 detHess 54.8
6.3027432764 × 12.5747526574 × 18.8551439832
25.1411233417 × 31.4354847149

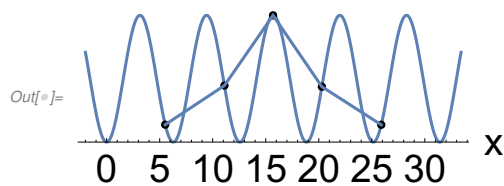


```
Barrier5 = 7.6467698
stat points SP1 node124 energy = 7.6467698 detHess - 2.12
point is anti - kink strong compressed chain
node124 = {5.5237908519, 11.1036633221, 15.6893717266,
20.2936706014, 25.8899560820};
```

```
node196 energy = 9.99458279 detHess 1.0 = SP2
node196 = {3.1415877789, 9.4031607659, 15.6863492641,
21.9911500834, 28.2959493944};
```

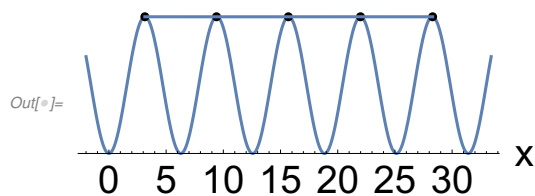
```
and node 264 and gMin node384
```

```
SetX = node124;
```



ok pull from SP1 results in moved gMin, without the SP2 ok
 first push moves 3 atoms to SP1
 second pull moves 3 last atoms to aim
 however PP goes symmetric over the central SP2 or higher !

```
SetX = node196;
```



```
N = 5 global minimum NoMisfit1
as = 6.283185307180;
a0 = as
Setxx = node196;
```

```
Out[*]= { {0., -1., 0, 0, 0}, {-1., 1., -1., 0, 0},
{0, -1., 1., -1., 0}, {0, 0, -1., 1., -1.}, {0, 0, 0, -1., 0.} }
```

```
In[*]= Eigenvalues[%]
```

```
Out[*]= {2.61803, 1.61803, -1., -0.618034, 0.381966}
```

```
### ## ## ## ## ## ## ## ## ## ## NoMisfit1 ### ## ## ## ## ## ## ## ## ##
```

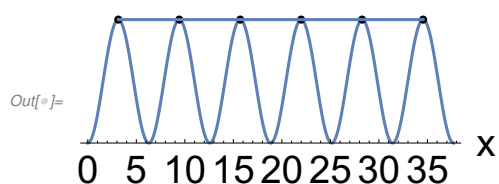
```
N = 6 global minimum No Misfit 1
```

In[*]:= Eigenvalues[%]

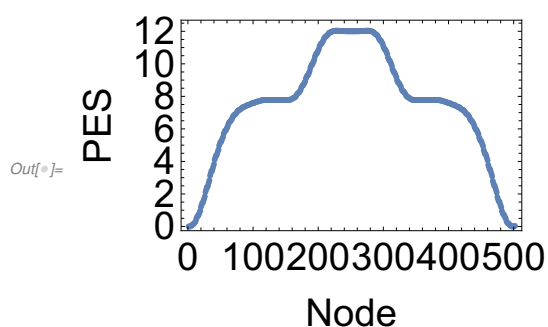
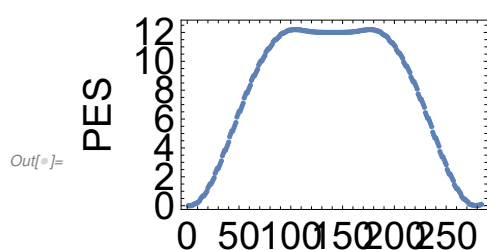
Out[*]:= {2.73205, 2., 1., -0.999999, -0.73205, 9.71749×10^{-7} }

SetX = {3.142986747947873`, 9.424777960769793`, 15.706569173591301`,
21.989754480770472`, 28.274333882307722`, 34.55891328384539`}

Out[*]:= {3.14299, 9.42478, 15.7066, 21.9898, 28.2743, 34.5589}



energy6D



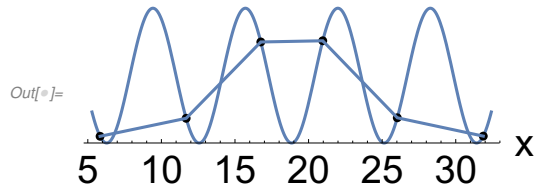
Barrier6 = 7.777998988

```
stat SP1 node144 energy = 7.777998988 detHess 0.496
node144 = {5.8341558868, 11.6818946348, 16.7560503583,
20.9637362511, 26.0273860801, 31.8710227894};
node254 flat energy = 11.9944617 detHess 5.28063
node254 = {3.1239158452, 9.4247808980, 15.7256430136,
22.0088263046, 28.2743327868, 34.5398403645 };
and node 360
```

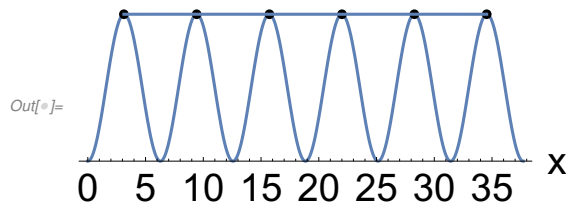
```

SetX = node144;
SetAA00 = Riffle[SetX, 1 - Cos[SetX]];
XXX = Partition[SetAA00, 2];
Bild = Show[Graphics[ {PointSize[0.02135], Black, Point[ XXX]}] , Fo

```



```
SetX = node254;
```



```

barrier6 = SP1 pull from SP1 goes to moved gMin ok
But it does not exist an iMin here

```

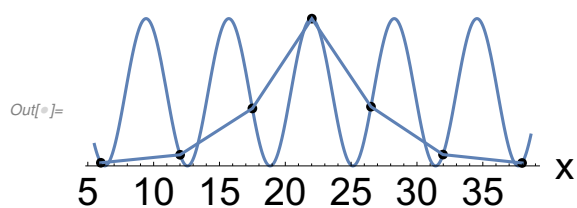
```
### ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##
```

```
N = 7 global minimum No Misfit 1
```

```

NoMisfit1 N = 7 SP Barrier7 = 7.8575085
SP node165 energy = 7.8575085 detHess - 8.11
node165 = {5.9904940568, 12.0096220046, 17.5003213139,
22.0154651761, 26.5062948336, 31.9777351302,
37.9818930967};
SetX = node165;

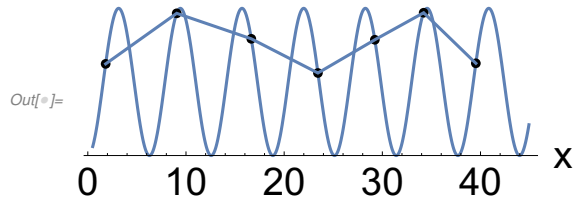
```



```

NoMisfit1 N = 7 SP asymmetric !
SP ? node282 energy = 13.5362183 detHess 1.626332
node282 = {1.8187439862, 9.0548841389, 16.6525407287,
23.4399479564, 29.2347875865, 34.2101755241,
39.5259647741};
SetX = node282;

```



```
Out[*] = {1.81665, 9.06976, 16.6705, 23.4506, 29.2369, 34.2025, 39.5158}
```

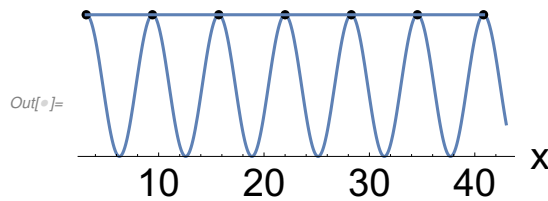
```
In[*] = Eigenvalues[%]
```

```
Out[*] = {3.33812, 2.53194, 1.91388, 1.09097, -0.556289, 0.440675, -0.37538}
```

```

iMin node324 energy = 13.99371648 detHess -0.99
node324 = {3.1305686944, 9.4137550690, 15.7079641122,
22.0021723112, 28.2853569974, 34.5575187917,
40.8296809838 };
SetX = node324;

```



```
Setxx = node324
```

```

Out[*] = {{0., -1., 0, 0, 0, 0, 0}, {-1., 1., -1., 0, 0, 0, 0},
{0, -1., 1., -1., 0, 0, 0}, {0, 0, -1., 1., -1., 0, 0},
{0, 0, 0, -1., 1., -1., 0}, {0, 0, 0, 0, -1., 1., -1.}, {0, 0, 0, 0, 0, -1., 0.}}

```

```
In[*] = Eigenvalues[%]
```

```
Out[*] = {2.80194, 2.24698, 1.44504, -1., -0.801938, 0.554958, -0.24698}
```

```

### ## ## ## ## ## ## ## ## ## ## NoMisfit1 ## ## ## ## ## ## ## ##
N = 8 global minimum NoMisfit1 start a0
as = 6.283185307180;
a0 = as

```

```
Out[*] = {3.14159, 9.42478, 15.708, 21.9911, 28.2743, 34.5575, 40.8407, 47.1239}
```

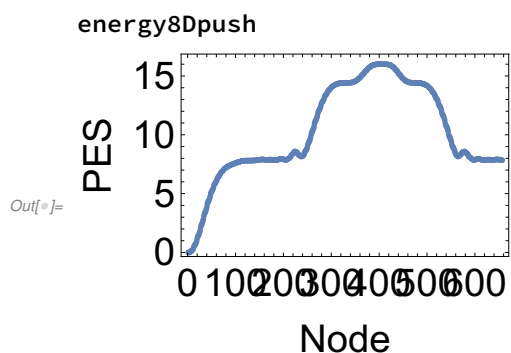
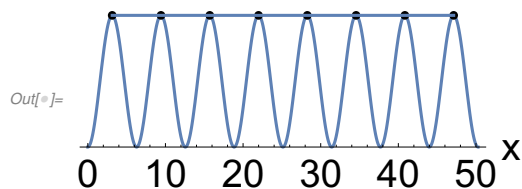
```

Out[*] = {{0., -1., 0, 0, 0, 0, 0, 0}, {-1., 1., -1., 0, 0, 0, 0, 0},
{0, -1., 1., -1., 0, 0, 0, 0}, {0, 0, -1., 1., -1., 0, 0, 0},
{0, 0, 0, -1., 1., -1., 0, 0}, {0, 0, 0, 0, -1., 1., -1., 0},
{0, 0, 0, 0, 0, -1., 1., -1.}, {0, 0, 0, 0, 0, 0, -1., 0.}}

```

```
Out[*] = {2.84776, 2.41421, 1.76537, 1., -1., -0.847759, -0.414214, 0.234633}
```

```
SetX = {3.141592653589386`, 9.424777960769793`,
        15.707963267949788`, 21.99114857512896`, 28.274333882307726`,
        34.55751918948691`, 40.8407044966669`, 47.123889803847305`}
```

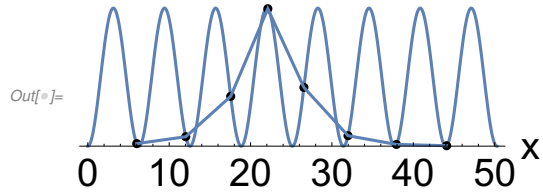


```
Barrier8 = 7.873142477
SP1 node 167 energy = 7.873142477 detHess - 17.982
6.0099496106 × 12.0375103989 × 17.5605215880
22.1229657665 × 26.5539741597 × 31.9738187824
37.9230626200 × 44.0943899209
node185 energy = 7.8559488451 detHess 16.563751
6.1235544971 × 12.2333895393 × 18.0163627738
23.0592534250 × 27.2258550541 × 32.2591220150
38.0391611546 × 44.1527338747
node206 energy = 7.873668326 detHess - 20.056434
6.1689753932 × 12.3429459222 × 18.2953459663
23.7214743338 × 28.1603005572 × 32.7129131257
38.2282734224 × 44.2484434873
node333 energy = 14.423259 detHess 1.896565125 SP2 ??
1.3088414447 × 8.5455689311 × 16.5525310877 ×
23.8118090535 × 30.1021409971 × 35.4253188130 ×
39.9855884022 × 45.3005050858 ×
node407 energy = 15.991438162 detHess - 1.00 SP3 ??
3.1415919611 × 9.4162412048 × 15.6994271008 ×
21.9911490605 × 28.2828705348 × 34.5660554603 ×
40.8407042186 × 47.1153532550 ×
and nodes 476 × 600 × 620
```

```

SP1 node167 energy = 7.873142477 detHess - 17.982
node167 = {6.0099496106, 12.0375103989, 17.5605215880,
22.1229657665, 26.5539741597, 31.9738187824,
37.9230626200, 44.0943899209};
SetX = node167;

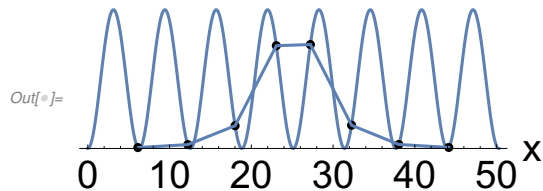
```



```

iMin node185 energy = 7.8559488451 detHess 16.563751
node185 = {6.1235544971, 12.2333895393, 18.0163627738,
23.0592534250, 27.2258550541, 32.2591220150,
38.0391611546, 44.1527338747};
SetX = node185;

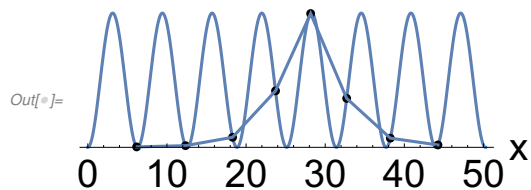
```



```

SP1 node206 energy = 7.873668326 detHess - 20.056434
node206 = {6.1689753932, 12.3429459222, 18.2953459663,
23.7214743338, 28.1603005572, 32.7129131257,
38.2282734224, 44.2484434873};
SetX = node206;

```



ok the MEP goes over this SP1 and iMin beginning with N = 8

```

### ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ## ##

```

```

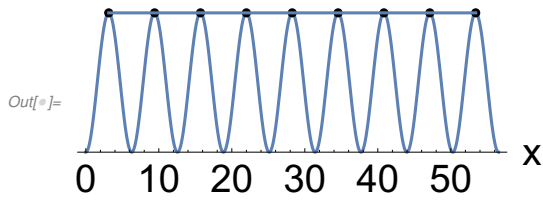
NoMisfit1 N = 9 SP start a0
Setxx = Table[a0 * (i - 1) + Pi, {i, 9}]

SetX = {3.140436941102519`, 9.424777960769656`, 15.709118980436518`,
21.992304287615962`, 28.274333882308138`, 34.55636347700031`,
40.83954878417976`, 47.12388980384662`, 53.40823082351376`}

```

In[*]:= Eigenvalues[%]

Out[*]:= {2.87939, 2.53209, 2., 1.3473, -1., -0.879385, 0.652704, -0.532088, 6.67836×10^{-7} }



NoMisfit1 N = 10 SP start a0

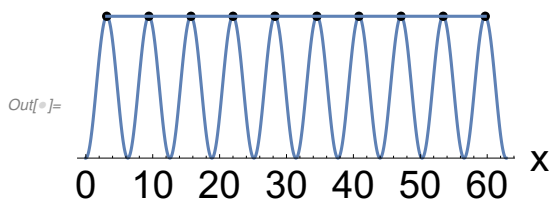
Setxx = Table[a0 * (i - 1) + Pi, {i, 10}]

Out[*]:= {3.14159, 9.42478, 15.708, 21.9911,
28.2743, 34.5575, 40.8407, 47.1239, 53.4071, 59.6903}

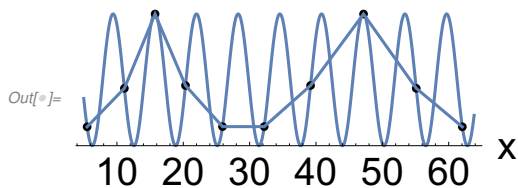
SetX = {3.123968103377397`, 9.424777048346987`, 15.72558690573897`,
22.008774037622054`, 28.274336619576136`, 34.53989646426223`,
40.82307812203441`, 47.12388524173331`, 53.4246969235458`, 59.70788770483666`}

In[*]:= Eigenvalues[%]

Out[*]:= {2.90222, 2.61813, 2.17566, 1.61815, 1.00011,
-0.999891, -0.901999, -0.617918, 0.382067, -0.175438}



SetX = node174;



NoMisfit1 N = 10 int SP

Setxx = node174;

Out[*]:= {5.51445, 11.1024, 15.6961, 20.3016,
25.9001, 32.1929, 39.1868, 47.1773, 55.1144, 62.0608}

Out[*]:= {{1.71879, -1., 0, 0, 0, 0, 0, 0, 0, 0, 0}, {-1., 2.10663, -1., 0, 0, 0, 0, 0, 0, 0, 0},
{0, -1., 1.00007, -1., 0, 0, 0, 0, 0, 0, 0}, {0, 0, -1., 2.11845, -1., 0, 0, 0, 0, 0, 0},
{0, 0, 0, -1., 2.71972, -1., 0, 0, 0, 0, 0}, {0, 0, 0, 0, -1., 2.71302, -1., 0, 0, 0, 0},
{0, 0, 0, 0, 0, -1., 2.08297, -1., 0, 0, 0}, {0, 0, 0, 0, 0, 0, -1., 1.00143, -1., 0, 0},
{0, 0, 0, 0, 0, 0, 0, -1., 2.13609, -1.}, {0, 0, 0, 0, 0, 0, 0, 0, -1., 1.71715}}

In[*]:= Eigenvalues[%]

Out[*]:= {4.27172, 3.48329, 3.27099, 2.93313, 2.12503,
1.50041, 1.09716, 0.894894, -0.154566, -0.107731}

NoMisfit1 N = 10 top SP of INDEX 4

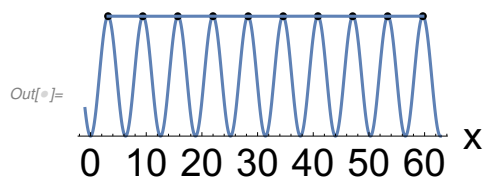
Setxx = node274;

Out[]:= $\left\{ \left\{ 1.67061 \times 10^{-6}, -1., 0, 0, 0, 0, 0, 0, 0, 0, 0 \right\}, \left\{ -1., 1., -1., 0, 0, 0, 0, 0, 0, 0, 0 \right\}, \right.$
 $\left. \left\{ 0, -1., 1., -1., 0, 0, 0, 0, 0, 0, 0 \right\}, \left\{ 0, 0, -1., 1., -1., 0, 0, 0, 0, 0, 0 \right\}, \right.$
 $\left. \left\{ 0, 0, 0, -1., 1., -1., 0, 0, 0, 0, 0 \right\}, \left\{ 0, 0, 0, 0, -1., 1., -1., 0, 0, 0 \right\}, \right.$
 $\left. \left\{ 0, 0, 0, 0, 0, -1., 1., -1., 0, 0 \right\}, \left\{ 0, 0, 0, 0, 0, 0, -1., 1., -1., 0 \right\}, \right.$
 $\left. \left\{ 0, 0, 0, 0, 0, 0, 0, -1., 1., -1. \right\}, \left\{ 0, 0, 0, 0, 0, 0, 0, 0, -1., 1.67061 \times 10^{-6} \right\} \right\}$

In[]:= Eigenvalues[%]

Out[]:= {2.90211, 2.61804, 2.17557, 1.61804, 1.,
 -0.999999, -0.902112, -0.618033, 0.381967, -0.175569}

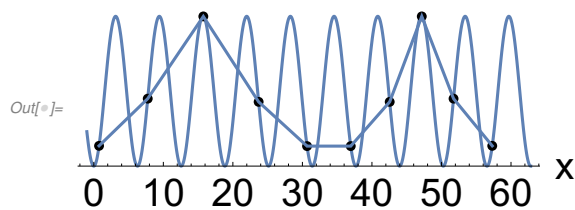
SetX = node274;



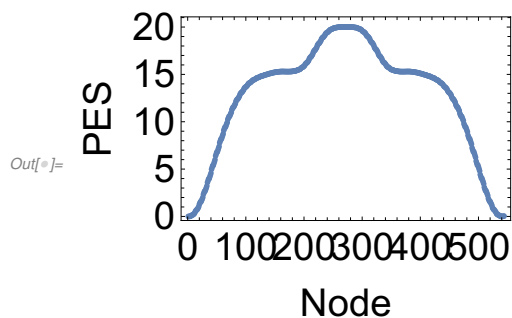
energy = 15.29406537 detHess 7.3777509

node371 = {0.7533025343, 7.7545559202, 15.7508753795,
 23.7042956939, 30.6678097952, 36.9510272944,
 42.5539837704, 47.1670720930, 51.7369909508,
 57.3020011367};

SetX = node371;



N = 10 NoMisfit1



```

stat points start energy 1.3788969965844444 E - 013 detHess 6763.5
0.00000000000 × 6.2831853072 × 12.5663706144 × 18.8495559215
25.1327412287 × 31.4159265359 × 37.6991118431 × 43.9822971503
50.2654824574 × 56.5486677646

```

```

SP1 node 174 energy = 15.294114 detHess 7.45
5.5071506028 × 11.1249159811 × 15.7510305087
20.3340906240 × 25.9134420663 × 32.1966117398
39.1835893766 × 47.1668553819 × 55.1071687279
62.0558173853

```

```

node 274 energy = 20.00000091 detHess 0.999997
3.1416060835 × 9.3814468210 × 15.6646052404
21.9911182013 × 28.3176406023 × 34.6008363620
40.8406995595 × 47.0805534794 × 53.3637392724
59.6902478422

```

```

node 371 energy = 15.29406537 detHess 7.3777509
0.7533025343 × 7.7545559202 × 15.7508753795
23.7042956939 × 30.6678097952 × 36.9510272944
42.5539837704 × 47.1670720930 × 51.7369909508
57.3020011367

```

```

node542 energy = 5.6196779563961741 E - 003 detHess 6748.59
6.3421301060 × 12.5889082534 × 18.8582228609
25.1362065637 × 31.4176583429 × 37.7008439903
43.9857632986 × 50.2741500630 × 56.5712060293
62.8908000571

```

```

node174 = {5.5071506028, 11.1249159811, 15.7510305087,
20.3340906240, 25.9134420663, 32.1966117398,
39.1835893766, 47.1668553819, 55.1071687279,
62.0558173853};

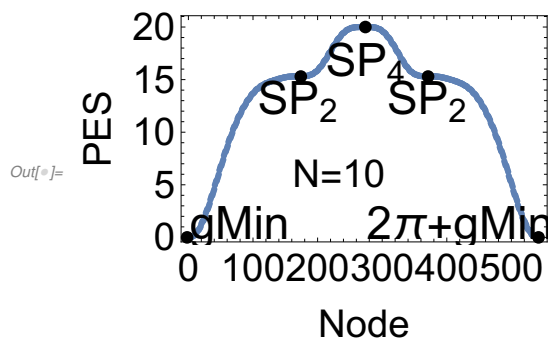
```

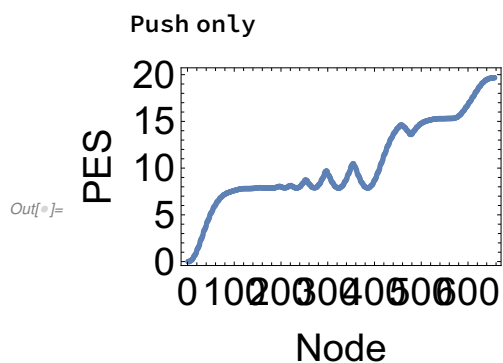
SP2 ?

```

node274 = {3.1416060835, 9.3814468210, 15.6646052404,
21.9911182013, 28.3176406023, 34.6008363620,
40.8406995595, 47.0805534794, 53.3637392724,
59.6902478422};

```





start energy 0.0

0.000000000 × 6.2831853072 × 12.5663706144 × 18.8495559215
 25.1327412287 × 31.4159265359 × 37.6991118431 × 43.9822971503
 50.2654824574 × 56.5486677646

SP node167 energy = 7.87607639 detHess - 120.9

5.9976158374 × 12.0426197492 × 17.5874138421
 22.1794242914 × 26.5842693732 × 31.9820375582
 37.9162153976 × 44.0658290330 × 50.2988935909
 56.5653711789

fully compressed o.k

node 184 energy = 7.86203895 detHess 126.54894

6.1638708653 × 12.2485766554 × 18.0208073522
 23.0559486202 × 27.2163775616 × 32.2481704990
 38.0194358101 × 44.1056119964 × 50.3148114250
 56.5733303132

node 209 energy = 7.8897720 detHess - 127.8

6.1490661676 × 12.3465731084 × 18.3260024217
 23.8053803649 × 28.3140243478 × 32.7829715817
 38.2314545198 × 44.1875937755 × 50.3476314215
 56.5897431759

node235 energy = 7.86866651 detHess 129.7

6.2891612522 × 12.4659111307 × 18.5423696008
 24.3164374987 × 29.3618569422 × 33.5217971060
 38.5419681701 × 44.3087308417 × 50.3962024140
 56.6140445115

node273 energy = 7.8937058 detHess - 128.0995

6.1669032849 × 12.4565429226 × 18.6365636765
 24.6051659640 × 30.0701867351 × 34.5598593515
 39.0471569517 × 44.5102684380 × 50.4773178062
 56.6546725802

node325 energy = 7.86811171 detHess 118.87

6.3601604940 × 12.5572528941 × 18.7452276050
 24.8290561368 × 30.6138137085 × 35.6796778464
 39.8444993403 × 44.8487355072 × 50.6150441046
 56.7238821997

```

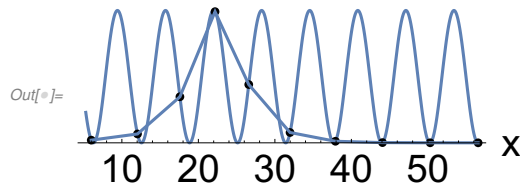
node387 energy = 7.882290 detHess - 128.18
6.1758233598 × 12.4989825168 × 18.7548015563
24.9159976940 × 30.8620957452 × 36.2820075073
40.7127806828 × 45.2712905931 × 50.7911465833
56.8129947736
node547 energy = 15.29380111 detHess 7.41840
0.7705961309 × 7.7171606277 × 15.6545637262
23.6453438882 × 30.6393391268 × 36.9321625308
42.5304301315 × 47.1336632143 × 51.7268845527
57.3156063796

```

```

SP node167 energy = 7.87607639 detHess - 120.9
fully compressed o.k
node167 = {5.9976158374, 12.0426197492, 17.5874138421,
22.1794242914, 26.5842693732, 31.9820375582,
37.9162153976, 44.0658290330, 50.2988935909,
56.5653711789};
SetX = node167;

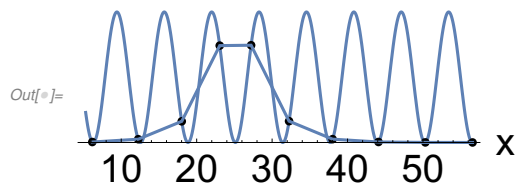
```



```

node184 energy = 7.86203895 detHess 126.54894
node184 = {6.1638708653, 12.2485766554, 18.0208073522,
23.0559486202, 27.2163775616, 32.2481704990,
38.0194358101, 44.1056119964, 50.3148114250,
56.5733303132};
SetX = node184;

```



SP node184 is iMin !

NoMisfit1 N = 10 of INDEX 0 !!!

```
Setxx = node184;
```

```

Out[*]:= {6.11186, 12.2246, 18.002, 23.0299,
27.196, 32.2432, 38.0266, 44.1317, 50.3856, 56.7594}

```

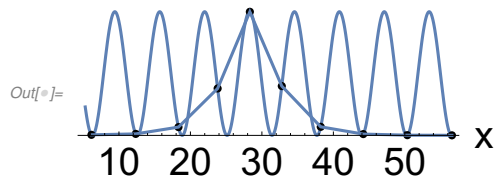
```
In[*]:= Eigenvalues[%]
```

```

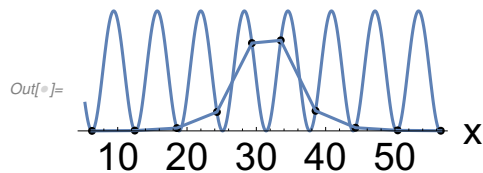
Out[*]:= {4.66548, 4.25155, 3.87055, 3.07092, 2.68864,
1.98689, 1.48806, 1.13213, 0.982657, 0.0556102}

```

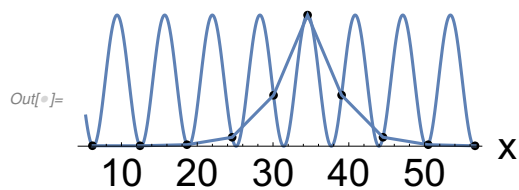
```
node 209 energy = 7.8897720 detHess - 127.8
node209 = {6.1490661676, 12.3465731084, 18.3260024217,
23.8053803649, 28.3140243478, 32.7829715817,
38.2314545198, 44.1875937755, 50.3476314215,
56.5897431759};
SetX = node209;
```



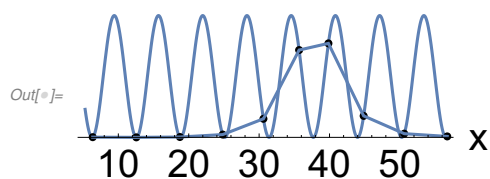
```
iMin next node235 energy = 7.86866651 detHess 129.7
node235 = {6.2891612522, 12.4659111307, 18.5423696008,
24.3164374987, 29.3618569422, 33.5217971060,
38.5419681701, 44.3087308417, 50.3962024140,
56.6140445115};
SetX = node235;
```



```
postSP1 node273 energy = 7.8937058 detHess - 128.0995
node273 = {6.1669032849, 12.4565429226, 18.6365636765,
24.6051659640, 30.0701867351, 34.5598593515,
39.0471569517, 44.5102684380, 50.4773178062,
56.6546725802};
SetX = node273;
```

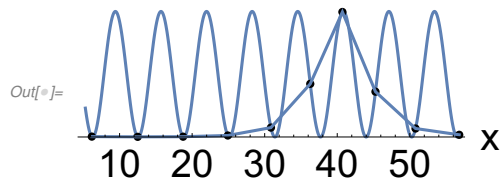


```
postliMin node325 energy = 7.86811171 detHess 118.87
node325 = {6.3601604940, 12.5572528941, 18.7452276050,
24.8290561368, 30.6138137085, 35.6796778464,
39.8444993403, 44.8487355072, 50.6150441046,
56.7238821997};
SetX = node325;
```

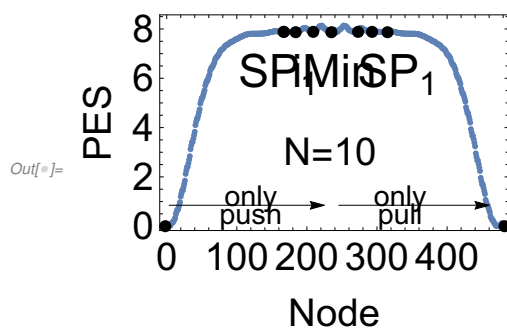


```
post2sp1 node387 energy = 7.882290 detHess - 128.18
node387 = {6.1758233598, 12.4989825168, 18.7548015563,
24.9159976940, 30.8620957452, 36.2820075073,
40.7127806828, 45.2712905931, 50.7911465833,
56.8129947736};
```

```
SetX = node387;
```



```
Join[NT10DNoMisfit1Push, NT10DNoMisfit1PullIMin]
```



```
### ### ### ### ### ### ### ### ### ### ### ### ### ### ### ### NoMisfit1
```

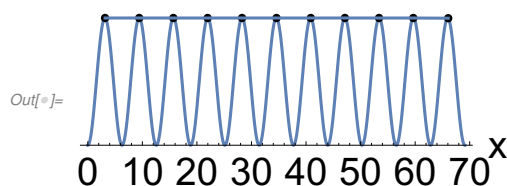
```
NoMisfit1 N = 11 global SP a0
```

```
Setxx = Table[a0 * (i - 1) + Pi, {i, 11}]
```

```
SetX = {3.168655191650987`, 9.424781263996794`,
15.680904033115185`, 21.964082735049747`, 28.274323972626878`,
34.584575119885265`, 40.867773637554194`, 47.12390631998157`,
53.38002248627428`, 59.6631879777208`, 66.05786381105727`}
```

```
In[*]:= Eigenvalues[%]
```

```
Out[*]:= {2.91924, 2.68281, 2.3101, 1.83121, 1.28514, -0.999447,
-0.918131, 0.715979, -0.681693, -0.308982, 0.169906}
```

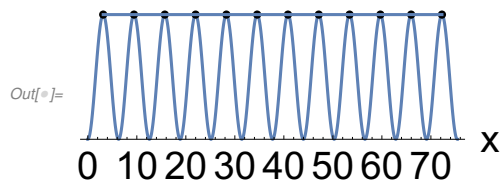


```
NoMisfit1 N = 12 global SP start a0
```

```
SetX = {3.1400438615146227`, 9.424777960769797`, 15.709512060024553`,
  21.992697367203718`, 28.27433388230772`, 34.55597039741214`,
  40.839155704592145`, 47.12388980384732`, 53.408623903102075`,
  59.691809210281235`, 65.97344572538525`, 72.25508224048967`}
```

```
In[*]:= Eigenvalues[%]
```

```
Out[*]:= {2.93185, 2.73205, 2.41421, 2., 1.51764, 1., -0.999999,
  -0.931851, -0.73205, 0.482363, -0.414213,  $1.19938 \times 10^{-6}$ }
```

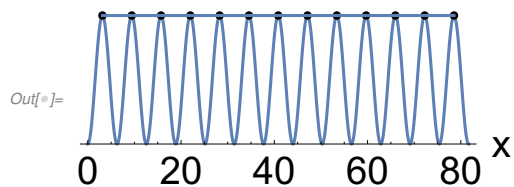


```
N = 13 NoMisfit1 global SP start a0
Setxx = Table[a0 * (i - 1) + Pi, {i, 13}]
```

```
SetX = {3.141592653589777`, 9.424777960769793`,
  15.707963267949395`, 21.991148575128566`,
  28.27433388230773`, 34.5575191894873`, 40.84070449666729`,
  47.1238898038473`, 53.407075111026906`, 59.690260418206094`,
  65.97344572538526`, 72.25663103256483`, 78.53981633974482`}
```

```
In[*]:= Eigenvalues[%]
```

```
Out[*]:= {2.94188, 2.77091, 2.49702, 2.13613, 1.70921, 1.24107, -1.,
  -0.941884, -0.770912, 0.758927, -0.497021, 0.29079, -0.136129}
```



Test only push - direction (1, 0, ... 0) for SP1?

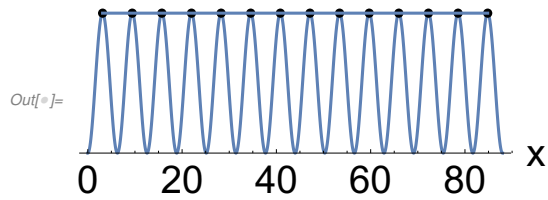
only pull von iMin aus

```
N = 14 NoMisfit1: global SP start a0
```

```
SetX = {3.1415926535894108`, 9.424777960769791`,
  15.707963267949761`, 21.99114857512894`, 28.274333882307737`,
  34.55751918948693`, 40.84070449666691`, 47.12388980384729`,
  53.407075111027275`, 59.69026041820648`, 65.97344572538528`,
  72.25663103256446`, 78.53981633974442`, 84.8230016469248`}
```

In[*]:= Eigenvalues[%]

Out[*]= {2.94986, 2.80194, 2.56366, 2.24698, 1.86777, 1.44504, -1., 1.,
-0.949856, -0.801938, -0.563663, 0.554958, -0.24698, 0.132233}



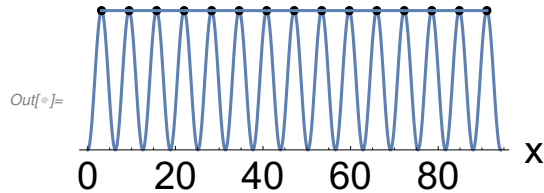
NoMisfit1 N = 15 local SP start mit a0

SetX = {3.1407509695642357`, 9.424777960769713`, 15.708804951974855`,
21.99199025915419`, 28.274333882307968`, 34.55667750546192`,
40.83986281264159`, 47.1238898038469`, 53.40791679505221`,
59.69110210223188`, 65.97344572538583`, 72.2557893485396`,
78.53897465571893`, 84.82300164692408`, 91.10702863812956`}

Out[*]= {3.14075, 9.42478, 15.7088, 21.992, 28.2743, 34.5567, 40.8399,
47.1239, 53.4079, 59.6911, 65.9734, 72.2558, 78.539, 84.823, 91.107}

In[*]:= Eigenvalues[%]

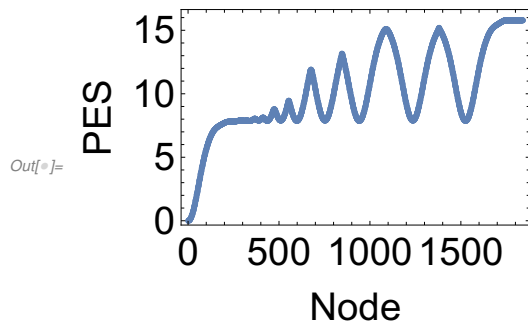
Out[*]= {2.9563, 2.82709, 2.61803, 2.33826, 2., 1.61803, 1.20906, -1., -0.956295,
-0.827091, 0.790943, -0.618034, 0.381966, -0.338261, 3.54216×10^{-7} }



*** ** ** ** **

N = 20 NoMisfit 1

NT20DPUSHpr0p04



o.k. the anti - kink wanders on equal high over alternating SP1 and iMin
 up to central symm iMin
 then we must use pull
 thus LEP is always ~ 7 units for all N
 the NT goes higher with TPs

```

start: en 0.0 detHess 102 333 063.7
0.000000000000 × 6.2831853072 × 12.5663706144 × 18.8495559215
25.1327412287 × 31.4159265359 × 37.6991118431 × 43.9822971503
50.2654824574 × 56.5486677646 × 62.8318530718 × 69.1150383790
75.3982236862 × 81.6814089933 × 87.9645943005 × 94.2477796077
100.5309649149 × 106.8141502221 × 113.0973355292 × 119.3805208364
SP1 node311 energy = 7.87592101 detHess - 1 857 820.78
6.0259343825 × 12.0429682998 × 17.5601723669
22.1167123823 × 26.5480182760 × 31.9672554008
37.9103121826 × 44.0630026830 × 50.2963111336
56.5604433773 × 62.8363509616 × 69.1167564205
75.3988799200 × 81.6816596535 × 87.9646900470
94.2478161870 × 100.5309789062 × 106.8141556168
113.0973377221 × 119.3805220203
iMin node342 energy = 7.860443717 detHess 1 883 888.12
6.1216058153 × 12.2260002460 × 17.9965488074
23.0138294780 × 27.1775865267 × 32.2311053891
38.0124743572 × 44.1021026087 × 50.3112502239
56.5661498049 × 62.8385306176 × 69.1175889651
75.3991979163 × 81.6817811112 × 87.9647364347
94.2478339023 × 100.5309856740 × 106.8141582141
113.0973387555 × 119.3805225324
node391 energy = 7.88953663 detHess - 1 887 588.98
6.1809537632 × 12.3574948343 × 18.3266756590
23.7964788631 × 28.2936593177 × 32.7715155398
38.2263039033 × 44.1842009079 × 50.3426326914
56.5781381966 × 62.8431098681 × 69.1193380980
75.3998660338 × 81.6820363166 × 87.9648339226
94.2478711507 × 100.530999217 × 106.8141636997
113.0973409553 × 119.3805236368
node438 energy = 7.86644357 detHess 2 035 425.93
6.2140847714 × 12.4351494491 × 18.5253692202
24.2970510339 × 29.3269732692 × 33.4881620193
38.5262424543 × 44.3003147443 × 50.3870712081
56.5951170527 × 62.8495954846 × 69.1218153984
75.4008122796 × 81.6823977515 × 87.9649719814
94.2479238923 × 100.5310200876 × 106.8141714558
113.0973440577 × 119.3805251881
node512 energy = 7.8920804 detHess - 1 875 473.59
6.2463779452 × 12.4870053522 × 18.6483507891
24.6098459296 × 30.0719504224 × 34.5596685238
39.0452372926 × 44.5056735450 × 50.4659171976

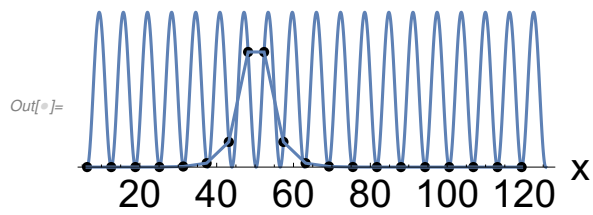
```

```

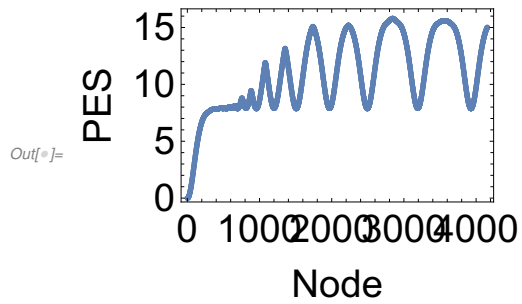
56.6252562365 × 62.8611088939 × 69.1262132002
75.4024920952 × 81.6830393862 × 87.9652170694
94.2480175214 × 100.5310558870 × 106.8141852248
113.0973495653 × 119.3805279419
node601 energy = 7.86777742 detHess 2 043 895.51
6.2602927763 × 12.5177644095 × 18.7266489749
24.8129358011 × 30.5848407678 × 35.6180820398
39.7786928059 × 44.8126407479 × 50.5847519033
56.6707360675 × 62.8784856104 × 69.1328507926
75.4050274464 × 81.6840078081 × 87.9655869817
94.2481588362 × 100.5311099191 × 106.8142060064
113.0973578779 × 119.3805320982
Barrier20 = 7.892400454
node755 energy = 7.892400454 detHess - 1 869 289.49
6.2790921272 × 12.5398364692 × 18.7740497795
24.9328286731 × 30.8930239379 × 36.3538222313
40.8399395942 × 45.3268218595 × 50.7882137377
56.7488541550 × 62.9083465747 × 69.1442579218
75.4093846540 × 81.6856721225 × 87.9662227071
94.2484016976 × 100.5312027779 × 106.8142417213
113.0973721639 × 119.3805392412
node944 energy = 7.868157615 detHess 1 958 861.68
6.2753025385 × 12.5481397763 × 18.8027471858
25.0105629512 × 31.0965041822 × 36.8684272274
41.9019570439 × 46.0625197272 × 51.0961068661
56.8680466304 × 62.9539632922 × 69.1616869381
75.4160422265 × 81.6882151123 × 87.9671940646
94.2487727780 × 100.5313446616 × 106.8142962919
113.0973939922 × 119.3805501553
node1239 energy = 7.892159436 detHess - 1 631 235.09
6.2646813246 × 12.5497685903 × 18.8182545947
25.0554443833 × 31.2154142757 × 37.1762128144
42.6376174739 × 47.1244777660 × 51.6107500959
57.0716984430 × 63.0321547227 × 69.1915759622
75.4274600805 × 81.6925764283 × 87.9688599789
94.2494091949 × 100.5315879975 × 106.8143898827
113.0974314284 × 119.3805688734
node1528 energy = 7.871943516 detHess 1 353 257.3030
6.2662258777 × 12.5540781571 × 18.8296382888
25.0852821045 × 31.2934846101 × 37.3795509026
43.1514674356 × 48.1848928973 × 52.3454729312
57.3791905884 × 63.1511923571 × 69.2371334439
75.4448664723 × 81.6992253765 × 87.9713997214
94.2503794345 × 100.5319589715 × 106.8145325650
113.0974885014 × 119.3805974099

SetX = node1528

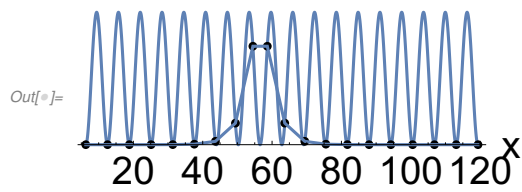
```



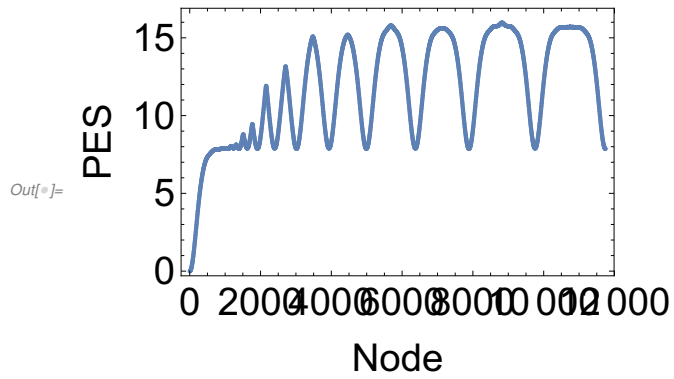
NT20DPUSH predictor 0.025



SetX = node3932;



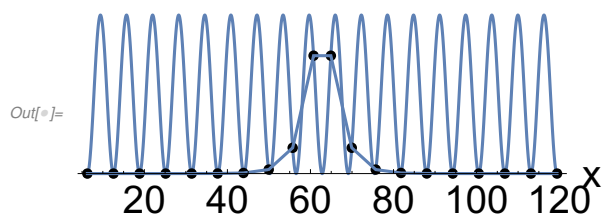
NT20DPUSH predictor 0.0125



```

last stat point node11745 energy = 7.8669656380 detHess 1 928 956.34
node11745 = {6.2821064477, 12.5651103798, 18.8468540778,
25.1258959353, 31.3980925528, 37.6524561327,
43.8601809266, 49.9460927777, 55.7180174642,
60.7515720638, 64.9121307047, 69.9456869504,
75.7176121171, 81.8035232626, 88.0112454110,
94.2656017505, 100.5377792894, 106.8167711500,
113.0983839354, 119.3810451270}
SetX = node11745

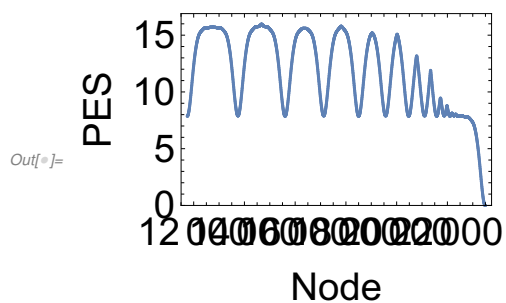
```



```

NT20DPULL iMin predictor 0.0125

```



```

last SP1 before desastre
node9760 energy = 7.892120025857 detHess - 1 909 089.94
6.2781235109 × 12.5630459455 × 18.8446437174
25.1213293050 × 31.3866032166 × 37.6225580109
43.7820337250 × 49.7425819409 × 55.2037349887
59.6902869567 × 64.1768123861 × 69.6379448384
75.5984776075 × 81.7579285608 × 87.9938244300
94.2589462666 × 100.5352345300 × 106.8157923954
113.0979924336 × 119.3808493760

```

higher stats

flat node 10566 energy = 15.658219395 detHess - 258.05

? BBP point crossed?

0.5079772615 7.3078652457 × 14.9623012322
 23.2951955349 × 30.6634569888 × 37.3482748228
 43.6894086955 × 49.7418236958 × 55.2941867476
 59.8961617475 × 64.2936872139 × 69.6852821726
 75.6167144141 × 81.7649031359 × 87.9964890241
 94.2599642285 × 100.5356237522 × 106.8159420964
 113.0980523140 × 119.3808793162
 node10706 energy = 15.684194214 detHess 16064.10
 0.2986599568 × 6.8768428861 × 14.0144223412
 22.1444781311 × 30.1218044543 × 37.1371615647
 43.6196811051 × 49.7474792722 × 55.3801311650
 60.0926043939 × 64.4135014076 × 69.7343395389
 75.6356439181 × 81.7721443088 × 87.9992555638
 94.2610211422 × 100.5360278681 × 106.8160975257
 113.0981144857 × 119.3809104021

node10791 energy = 15.682926224 detHess - 18054.41

0.2922856954 × 6.8652345042 × 13.9879201746
 22.0994892044 × 30.1029294253 × 37.1394162302
 43.6449747553 × 49.8195717054 × 55.5628888993
 60.4725036496 × 64.6772460080 × 69.8445230252
 75.6782855604 × 81.7884632081 × 88.0054907035
 94.2634032027 × 100.5369386614 × 106.8164478311
 113.0982546079 × 119.3809804632

node flat 10931 energy = 15.65036411 detHess 5196.76

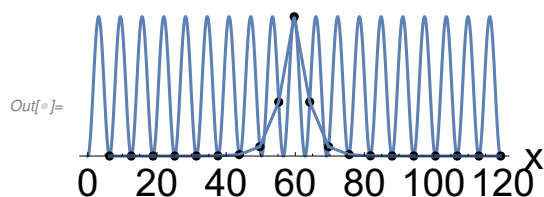
0.4773255769 × 7.2747660200 × 14.9090987179
 23.2599959689 × 30.6561344938 × 37.3635023239
 43.7415254091 × 49.8810963172 × 55.6456770837
 60.6250754092 × 64.7999845322 × 69.8969891253
 75.6986586106 × 81.7962637739 × 88.0084713640
 94.2645419403 × 100.5373740644 × 106.8166152940
 113.0983215930 × 119.3810139557

node 11747 energy = 7.867617657 detHess 1928472.7288

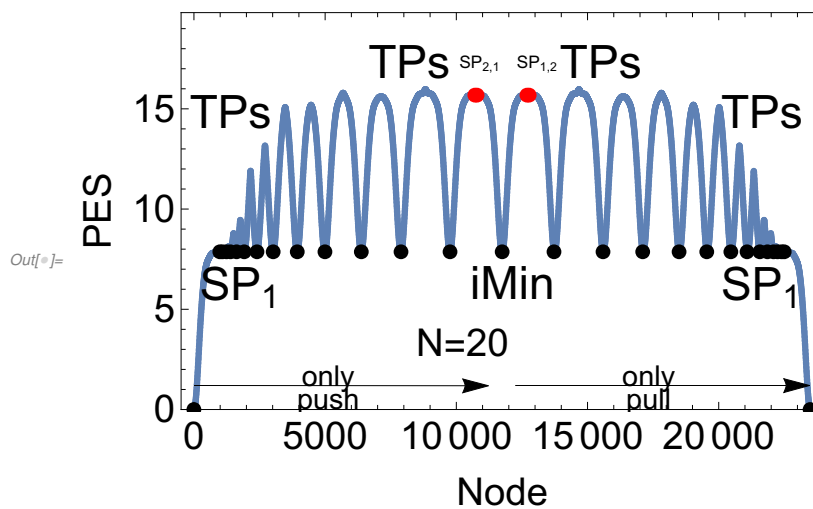
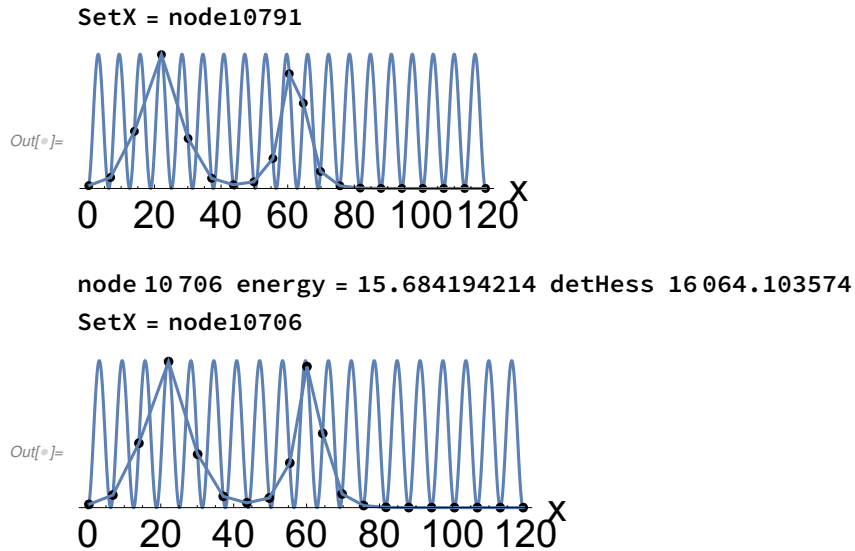
last SP1 before desastre

node 9760 energy = 7.892120025857 detHess - 1909089.94

SetX = node9760



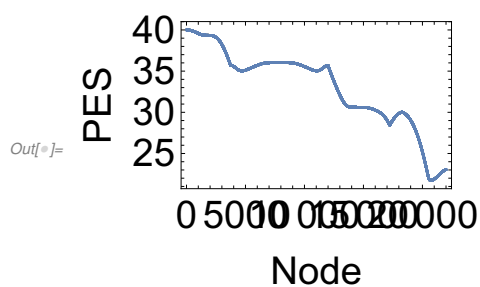
node10791 energy = 15.682926224 detHess - 18054.41



```
Setxx = Table[a0 * (i - 1) + Pi, {i, 20}];
```

```
Out[f*]= {3.14159, 9.42478, 15.708, 21.9911, 28.2743, 34.5575,
40.8407, 47.1239, 53.4071, 59.6903, 65.9734, 72.2566, 78.5398,
84.823, 91.1062, 97.3894, 103.673, 109.956, 116.239, 122.522}
```

```
start at NT20DcentralSPindex7
```



stat points

```
node 1743 energy = 39.350058432 detHess 3.6
4.2330378647 × 9.6275973263 × 14.8207249671
20.7891831926 × 27.6903908922 × 35.1429164239
42.0429113067 × 48.0100690239 × 53.2025649923
58.5981485038 × 64.8813336813 × 72.0521205875
79.4259953505 × 86.0252085200 × 91.6915844986
96.8054295575 × 102.4705922105 × 109.0685043537
116.4417472987 × 123.6135586516
node7874 energy = 36.06163396 detHess - 1.03
1.3118621109 × 8.5618021471 × 16.5715235979
23.8210841818 × 30.1040318379 × 35.4203069910
39.9769233975 × 45.2938446761 × 51.5773493454
58.8275186596 × 66.8373166179 × 74.0867521742
80.3696224927 × 85.6858445014 × 90.2423701640
95.5592231959 × 101.8426350907 × 109.0926643449
117.1025417366 × 124.3522235352
node14815 energy = 30.587395 detHess 77.31
5.5191513157 × 11.1095819664 × 15.7065035972
20.3048848987 × 25.8966083201 × 32.1800526426
39.1554036156 × 47.1242061712 × 55.0926923632
62.0677593641 × 68.3509433467 × 73.9422426153
78.5401168110 × 83.1376905066 × 88.7287167234
95.0116466184 × 101.9862973764 × 109.9542909611
117.9237364601 × 124.8996742841
```

```

stat point node = 12 227 energy = 23.3912652315 detHess - 255.63
5.6576085728 × 11.3533913687 × 16.1125105854
20.4780271436 × 25.8418809661 × 31.8569159281
38.2987853009 × 45.3050276100 × 53.2806590403
61.3823701007 × 68.4914306060 × 75.0165234500
81.1691174121 × 86.8315354460 × 91.5882404334
95.8813457944 × 101.1724817745 × 107.0620291752
113.1969248714 × 119.4312453697
node = 12 487 energy = 23.3909482 detHess 238.46
5.6591384868 × 11.3600404575 × 16.1266282500
20.4866749425 × 25.8445230912 × 31.8555552721
38.2921909871 × 45.2877436696 × 53.2482971760
61.3669623145 × 68.4912302082 × 75.0313677739
81.2128230090 × 86.9426531026 × 91.8193608235
96.0418311189 × 101.2394833168 × 107.08784449833
113.2064971611 × 119.4340943002
node = 16 620 energy = 23.44333299 detHess - 492.97
5.6668321214 × 11.3704543337 × 16.1435249949
20.4946759079 × 25.8430660890 × 31.8435363682
38.2587036807 × 45.2047113292 × 53.0906452189
61.2877547989 × 68.4852207507 × 75.0936893159
81.4023088778 × 87.4354377418 × 92.9637611715
97.5329243322 × 101.9590279485 × 107.3749624503
113.3227711394 × 119.4941107997
node = 17 436 energy = 23.4374986 detHess 256.65
5.7015055076 × 11.4374250638 × 16.2693828245
20.5689521963 × 25.8575008981 × 31.8090051361
38.1435434082 × 44.9080264156 × 52.4715688712
60.8400109168 × 68.2957909683 × 75.0209388295
81.3776890429 × 87.4353672983 × 92.9881793112
97.5890232948 × 101.9915399700 × 107.3879884281
113.3272963414 × 119.4945436223

```

N = 20 a0 NoMisfit1 as PP direction goes over other SP of index ?

SPweg20DPP

