You can do it with Dirax

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Our target for today....

Do simple cells with Dirax

```
1.54056
 18.750    25.940    24.090        130.8
 17.090   -82.500    38.660        112.3
 18.750  -158.090    18.740        141.7
 14.680  -158.740    24.920        194.5
 15.060   150.870    48.900         99.2
 14.690   145.530    50.810         82.0
 15.050    82.250    51.910         87.8
....
```

Do simple cells with Dirax

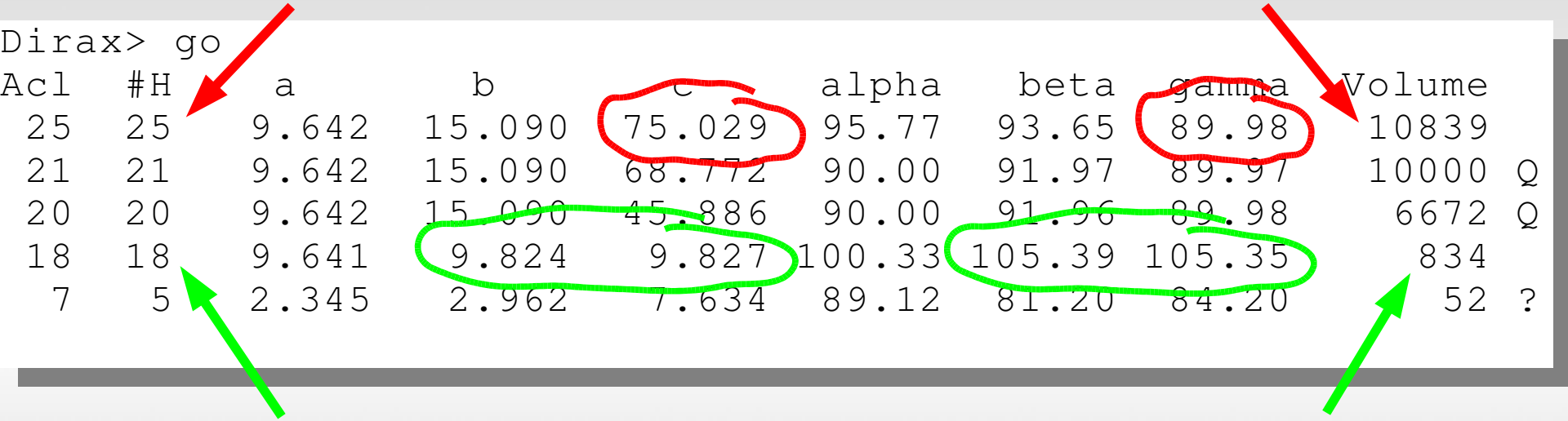
```
1.54056
Dirax> go
Acl   #H     a        b        c      alpha   beta   gamma  Volume

 25   25    6.530   41.209    6.671   89.99 101.53   90.00   1759
 13   13    6.530    6.671   10.431   88.22  80.99   78.48    440 Q
  9    9    6.530    6.671    8.410   97.33  97.10  101.54    352 ?
  8    8    5.893    6.519    6.529  116.29 113.09   95.59    195
  7    7    4.930    5.173    6.530   91.48 104.10   97.39    160 ?
selected ACL 25
```

Do simple cells with Dirax

```
 1.54056
Dirax> go
Acl   #H     a         b         c       alpha    beta   gamma   Volume

 25   25    6.530   41.209    6.671   89.99 101.53   90.00   1759
 13   13    6.530    6.671   10.431   88.22  80.99   78.48    440 Q
  9    9
  8    8                                                      195
  7    7                                                      160 ?
selected
```

```
Dirax> cell
cell for ex00
a, b, c :    6.5298   41.2087    6.6705
al,be,ga:   89.993   101.527   89.997
  volume: 1758.721
Nrefls=25 Nfit=25 Nnonfit=0
```

Do twinned cells with Dirax



```
Dirax> go
Acl   #H      a        b        c       alpha    beta   gamma   Volume
 25   25    9.642   15.090   75.029   95.77   93.65   89.98    10839
 21   21    9.642   15.090   68.772   90.00   91.97   89.97    10000 Q
 20   20    9.642   15.090   45.886   90.00   91.96   89.98     6672 Q
 18   18    9.641    9.824    9.827  100.33  105.39  105.35      834
  7    5    2.345    2.962    7.634   89.12   81.20   84.20       52 ?
```

Do twinned cells with Dirax

```
Dirax> go
Acl   #H     a        b        c      alpha    beta   gamma   Volume
 Dirax> acl 18
 selected ACL 18
 Dirax> lchi
 Nfit:7          123456789 123456789 12345
QNonfit:18       nHnnnnHHHnHnnnnnnnHHnnnnnn
 Dirax> go
Q7 H_reflections selected out of 25
 Acl   #H     a        b        c      alpha    beta   gamma Volume
   7   10    9.643    9.821    9.826 100.35 105.36 105.34    834

?
```

Do twinned cells with Dirax

```
Dirax> go
Acl  #H     a        b        c      alpha    beta   gamma   Volume
 Dirax> acl 18
Dirax> compare a b
Correlation=-0.77
         a        b        c       alpha     beta    gamma   volume
 A :   9.641    9.824    9.827   100.33   105.39   105.35    833.7
 B :   9.643    9.821    9.826   100.35   105.36   105.34    833.6
Volume ratio = 1.0 Trying 216 solutions
Nr Rotangl  Rotvec(xyz)     RotVec(hkl)     RotVec(uvw)      Fom
 1 -179.95  0.19 0.39 0.90 11.0 -2.9 -2.9 1.0  0.0  0.0   0.150
 2  179.99  0.77-0.62 0.10  0.0  1.0  1.0 7.0 12.9 13.0   0.130
Selected Solution 2

H'= -1.000*H +0.000*K +0.000*L
K'= +0.539*H -0.001*K +0.999*L
L'= +0.540*H +1.000*K +0.001*L   abaaaabbbabaaaaaabbaa***a
```

Do modulated cells with Dirax

```
Dirax> go
Acl   #H      a         b         c       alpha    beta   gamma  Volume
 25   25    4.413    20.713    25.766    90.76   94.87   96.11    2333 ?
 24   24    4.413    18.116    20.714    99.18   96.12   96.92    1609 ?
 21   25    4.413    18.109    20.713    99.22   96.11   96.86    1609 ?
 16   16    4.219     5.069     4.219    89.95  116.94   90.01      80 Q
 11   11    3.827     4.414     5.440    68.71   82.90   70.02      80 ?
  9    9    2.350     3.760     5.177    89.89   78.25   89.36      45 ?
selected ACL 16
```

Do modulated cells with Dirax

```
Dirax> go
Acl Dirax> lon                                                    Volume
       nr        H       K        L   1/err Netint
 25 Nn  1: -0.203 1.447  1.203     10  453.0   2333 ?
 24 Nn  9: -1.205 1.447  0.205     10  190.0   1609 ?
 21 Nn 10:  0.795 2.447 -1.796     10  222.0   1609 ?
 16 Nn 15:  0.408 3.104  0.593      9   84.0     80 Q
 11 Nn 17:  0.204 2.553  0.796     10  502.0     80 ?
  9 Nn 19: -1.204 2.446  0.204     10  294.0     45 ?
sel Nn 21:  1.796 2.448 -0.797     10  312.0
    Nn 22: -0.204 2.450  1.205      9  342.0
    Nn 25:  0.204 1.552  0.796     10  373.0
```

Do modulated cells with Dirax

```
Dirax> go
Acl
Dirax> lon
      nr        H      K       L   1/err Netint
 25 Nn  1: -0.203 1.447   1.203     10   453.0
 24 Nn  9: -1.205 1.447   0.205     10   190.0
 21 Nn 10:  0.795 2.447  -1.796     10   222.0
 16 Nn 15:  0.408 3.104   0.593      9    84.0
 11 Nn 17:  0.204 2.553   0.796     10   502.0
  9 Nn 19: -1.204 2.446   0.204     10   294.0
sel Nn 21:  1.796 2.448  -0.797     10   312.0
    Nn 22: -0.204 2.450   1.205      9   342.0
    Nn 25:  0.204 1.552   0.796     10   373.0
```

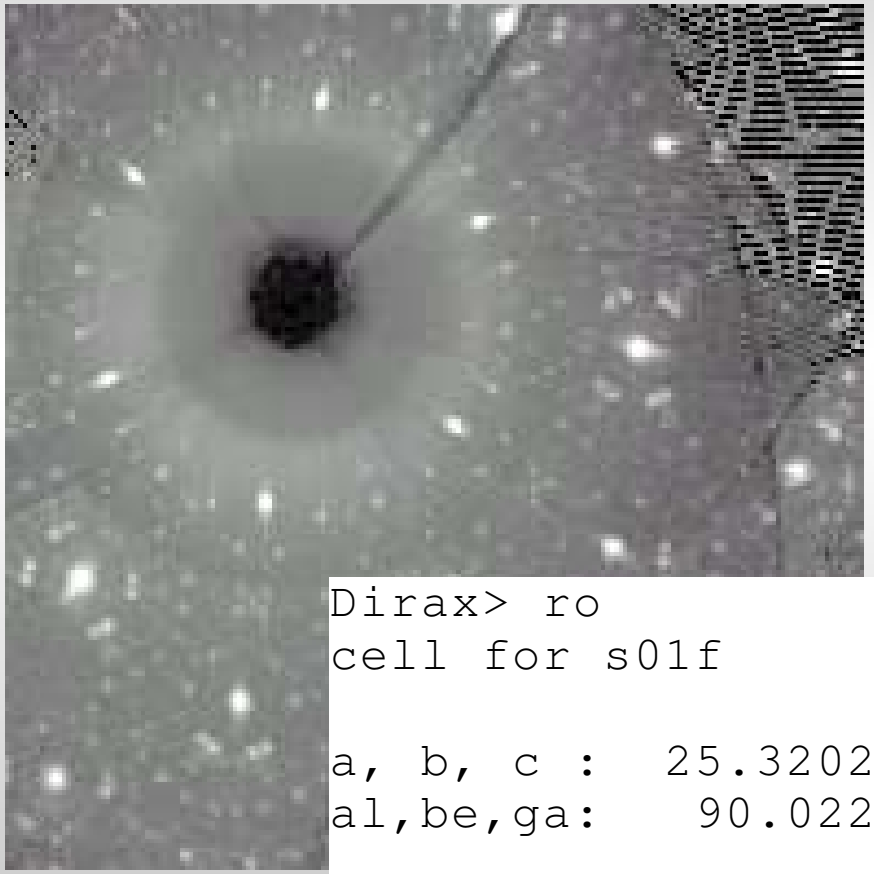
```
Volume
2333 ?
1609 ?
1609 ?
  80 Q
  80 ?
  45 ?
```

```
Dirax> qvtest
 qv nhit qvector
  1    8 -0.2040  0.4475  0.2040
```

Do modulated cells with Dirax

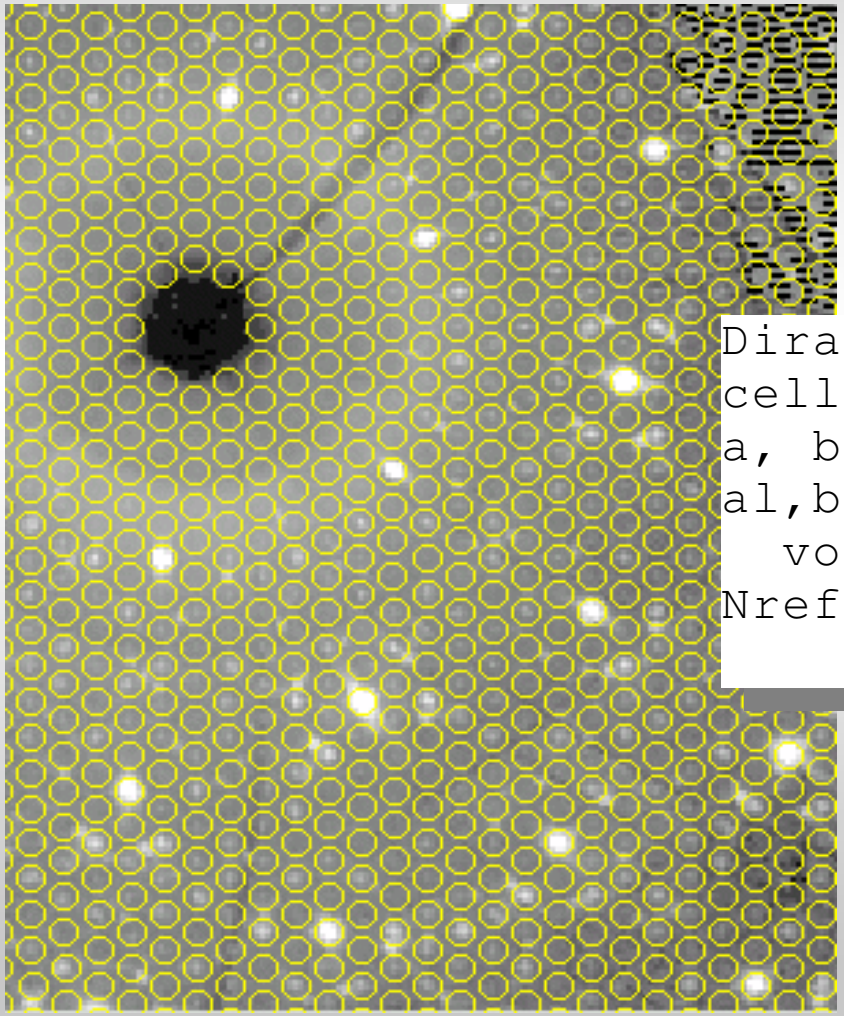
```
Dirax> sethklm
qvector= -0.204 0.447 0.204
Refl    h        k        l     order    h        k        l
   1 -0.2032   1.4472   1.2027     1   0.0008   0.9997   0.9987
   9 -1.2045   1.4472   0.2047     1  -1.0005   0.9997   0.0006
  10  0.7955   2.4470  -1.7958     1   0.9995   1.9995  -1.9999
  17  0.2039   2.5534   0.7959    -1  -0.0001   3.0009   0.9999
  19 -1.2039   2.4460   0.2042     1  -0.9999   1.9985   0.0002
  21  1.7956   2.4483  -0.7966     1   1.9996   2.0008  -1.0007
  22 -0.2038   2.4496   1.2048     1   0.0002   2.0021   1.0008
  25  0.2039   1.5520   0.7957    -1  -0.0001   1.9994   0.9997
Dirax> lon
    nr      H      K      L  M 1/err  Netint
Nn 15: 0.408 3.104 0.593 0      9   84.0
Dirax> qvorder 2
Dirax> sethklm
qvector= -0.204 0.447 0.204
Refl    h        k        l     order    h        k        l
  15  0.4077   3.1044   0.5928    -2  -0.0004   3.9994   1.0009
```

Do impossible cells with Dirax



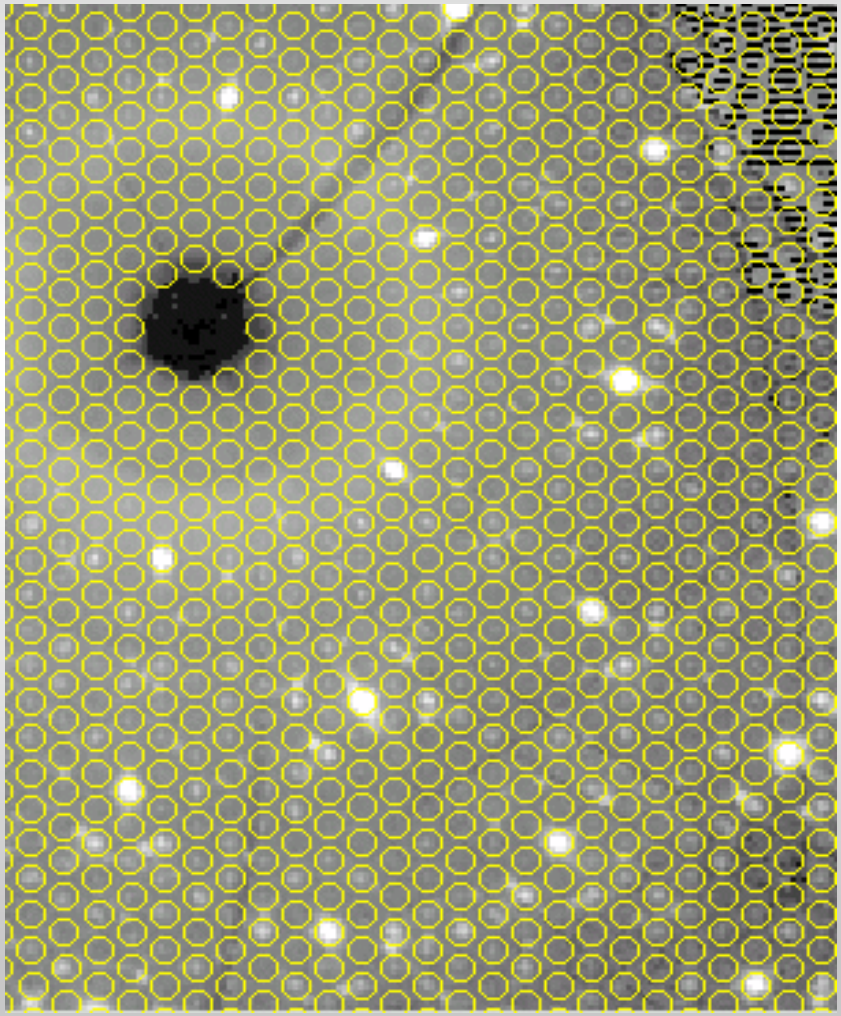
```
Dirax> ro
cell for s01f

a, b, c :  25.3202  16.1250 25.3788
al,be,ga:   90.022  119.850  89.973

  volume: 8987.186
Nrefls=1000 Nfit=494 NNonfit=506
```

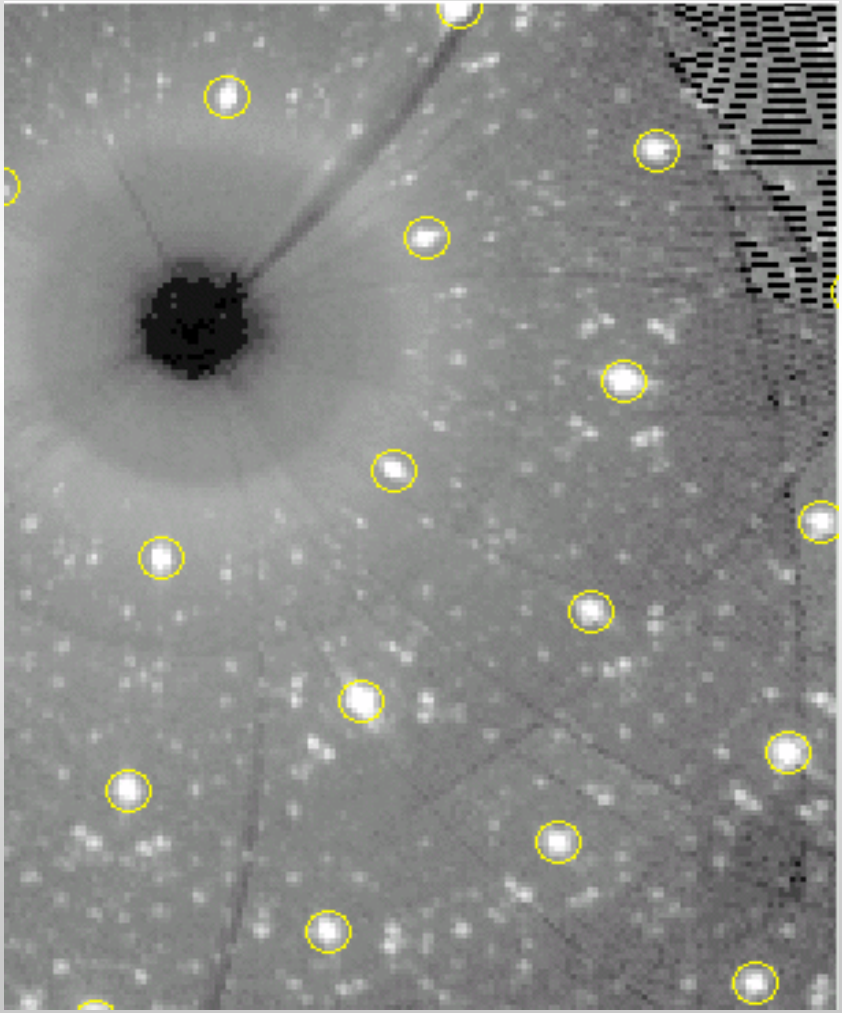
Do impossible cells with Dirax



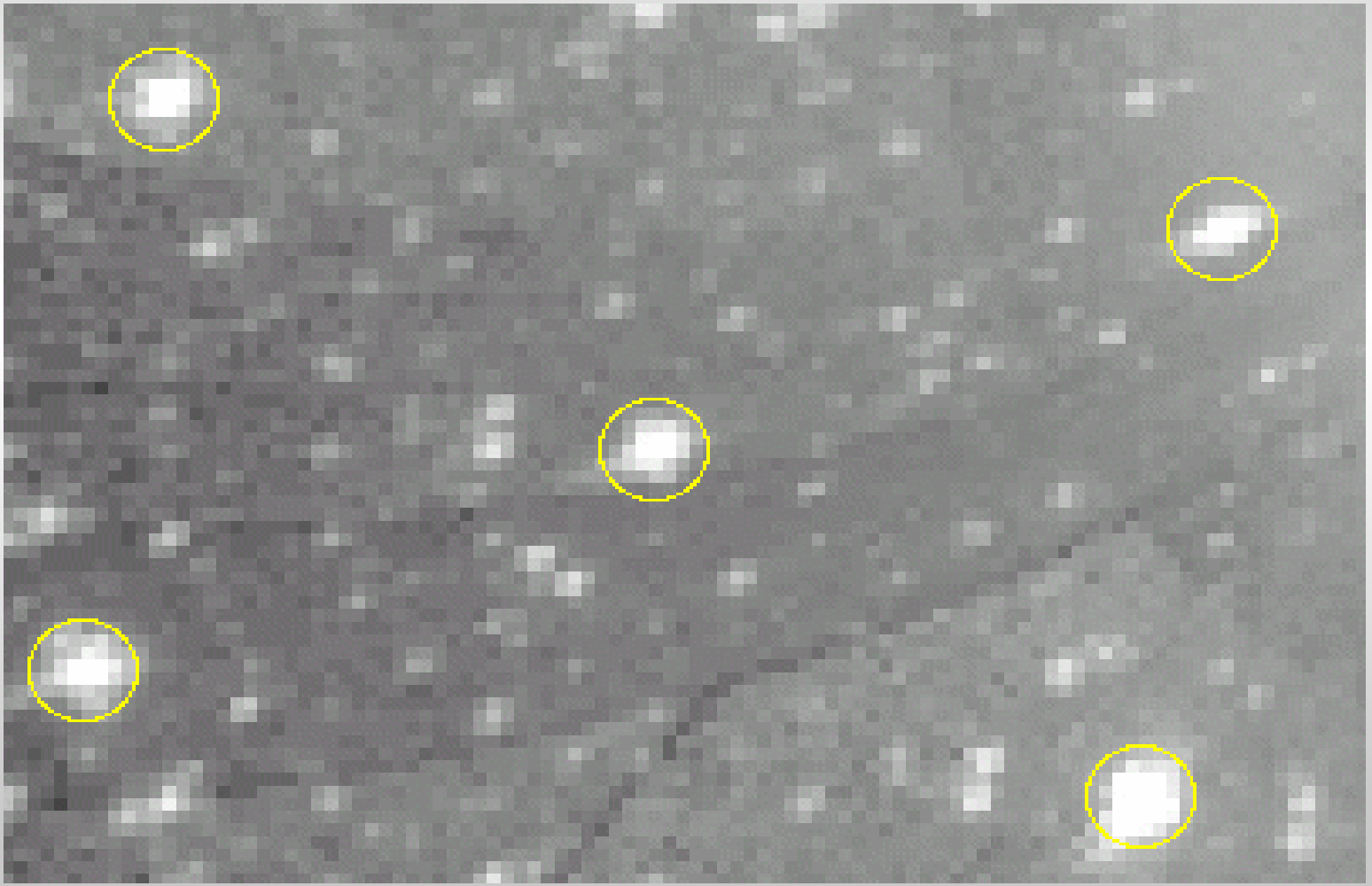
```
Dirax> ro
cell for strong
a, b, c :    3.8562   16.0947   3.8598
al,be,ga:    89.992   119.765   89.949
  volume: 207.9514
Nrefls=45 Nfit=45 NNonfit=0
```

Do impossible cells with Dirax

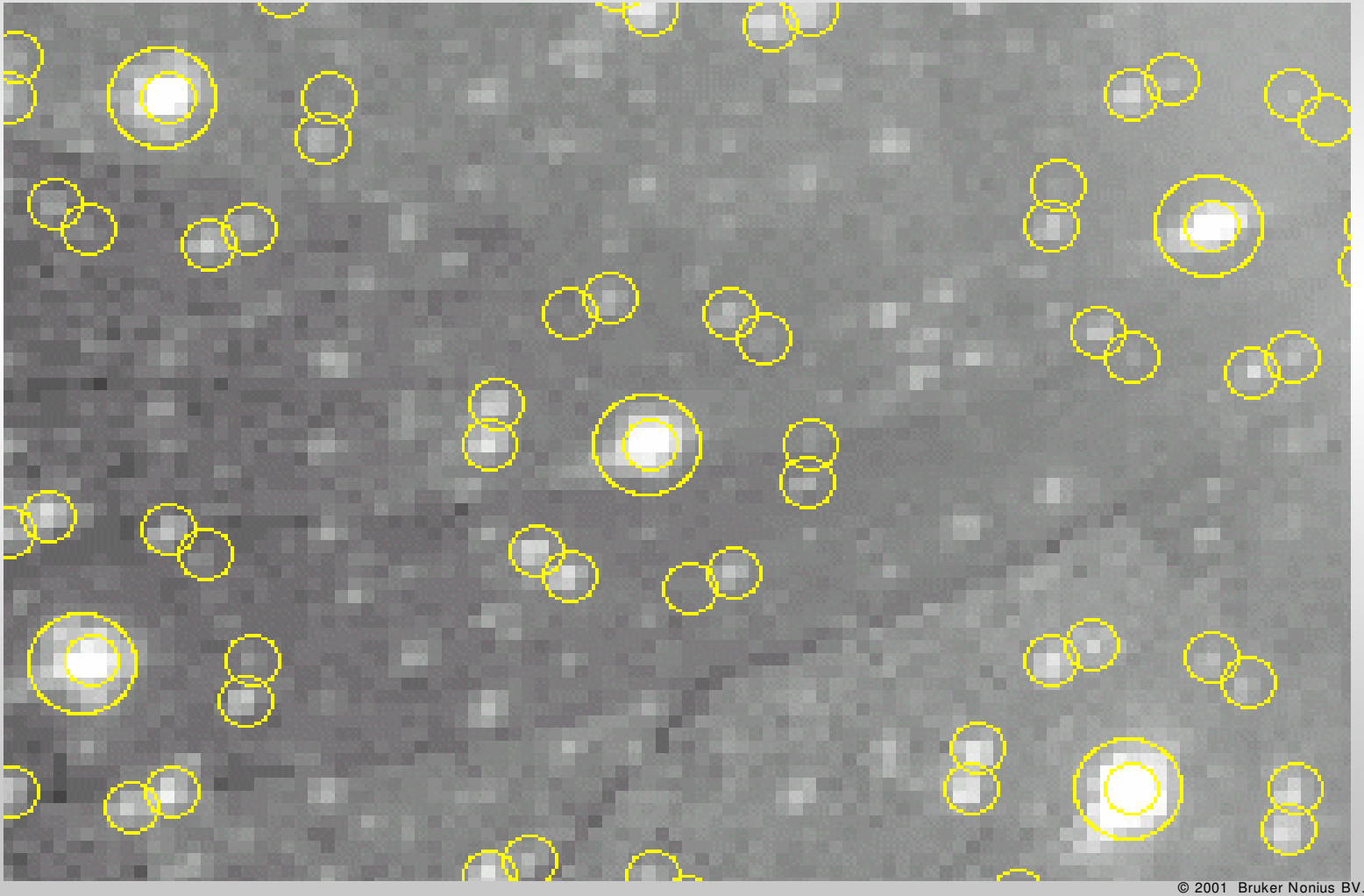




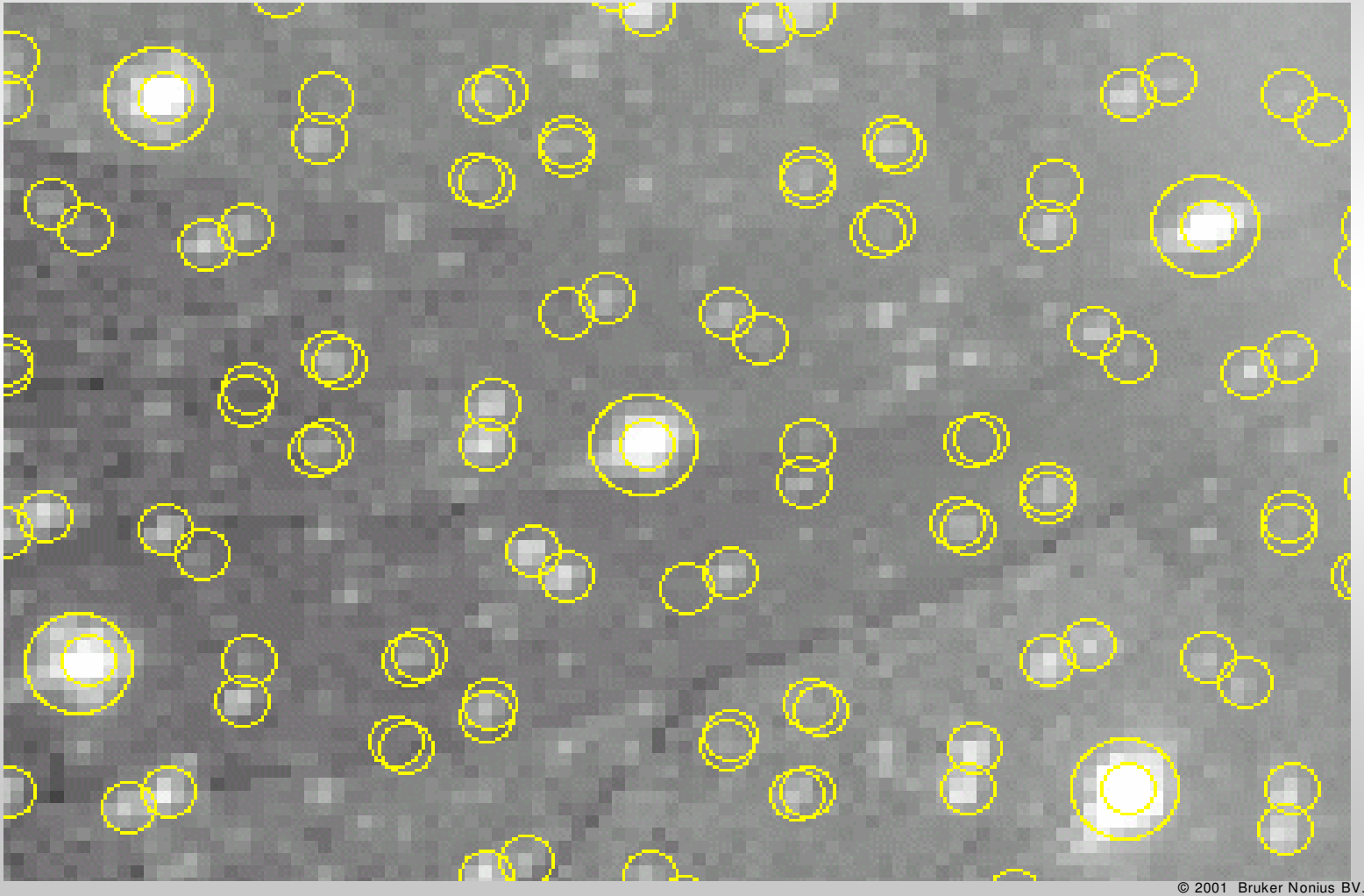
Do impossible cells with Dirax



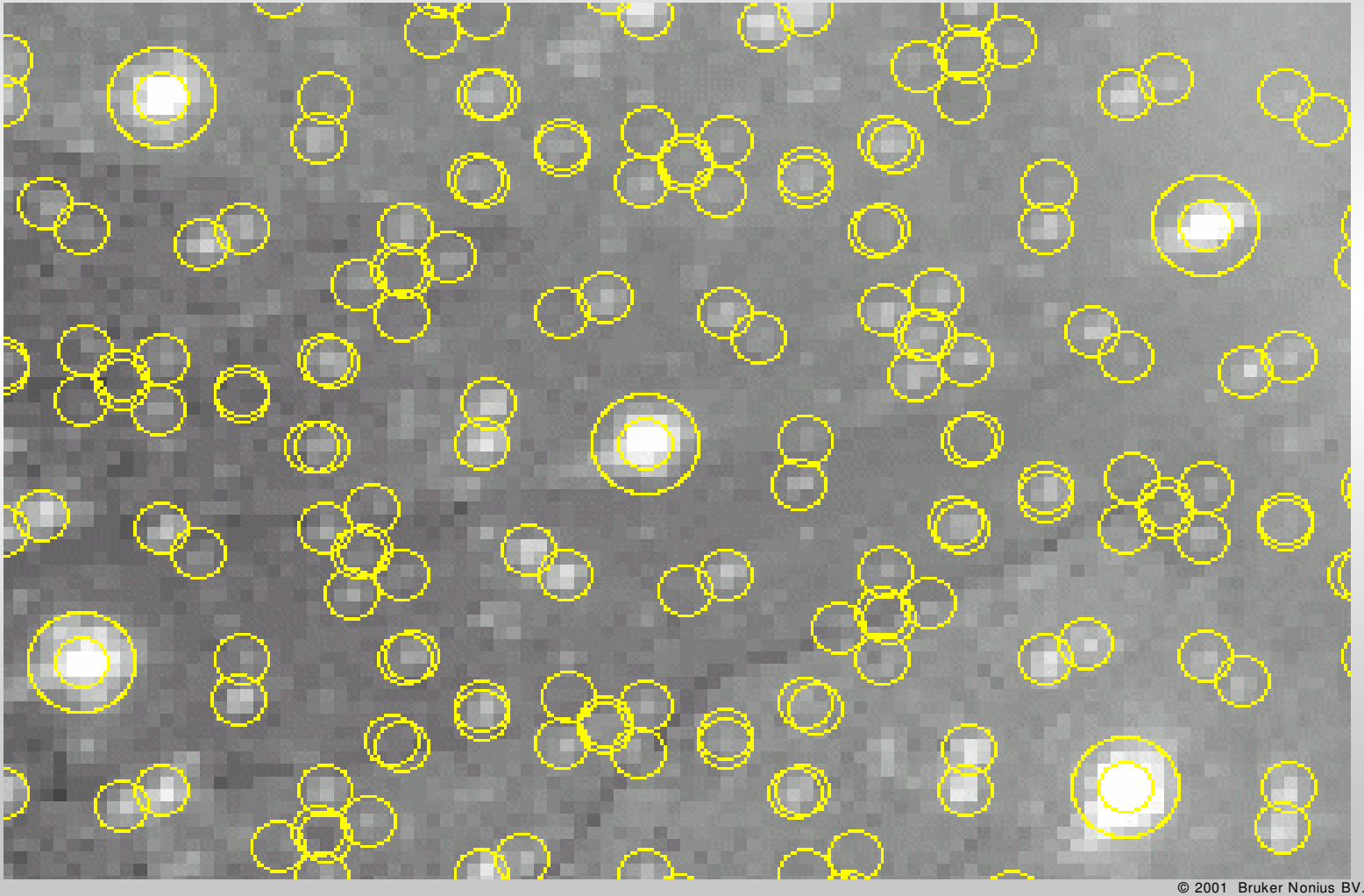
Do impossible cells with Dirax



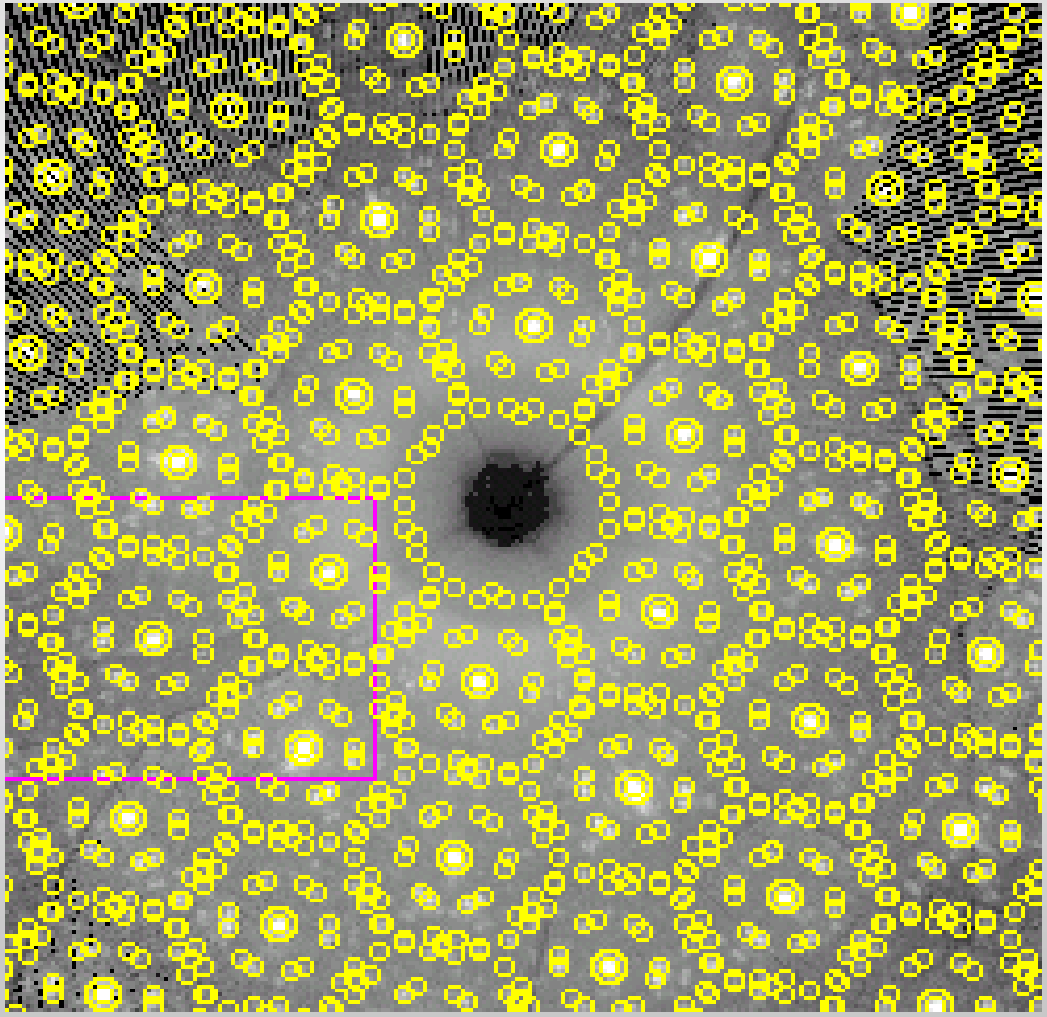
Do impossible cells with Dirax



Do impossible cells with Dirax



Conclusion



You can do it with Dirax!