SEP4 Status: HKL Integration

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Diffractometer control from Sardana using the Hkl Library from F. Picca (Soleil)

Sardana Workshop
DESY, 06-09-15

Documentation and code

- SEP with documentation since June 2013 (DRAFT)
- Dedicated Fork from Sardana Repository since August 2013

Details of the implementation

- Sardana controller (PseudoMotor) implementing the diffractometer (in Fork)

  Use of the hkl library exclusively done in hkl controller code,
  not in Sardana core

- Dedicated sardana macros (not in Fork)
- Dedicated Taurus GUIs (not in Fork)

Tests and perfomance

- Sardana controller:
  - tested during last year (performance and completeness)
  - used at Petra and LPS (Orsay)

- HKL macros:
  - developed by request of the beamline scientists
  - offers full control and info of the diffractometer
  - used at Petra and LPS

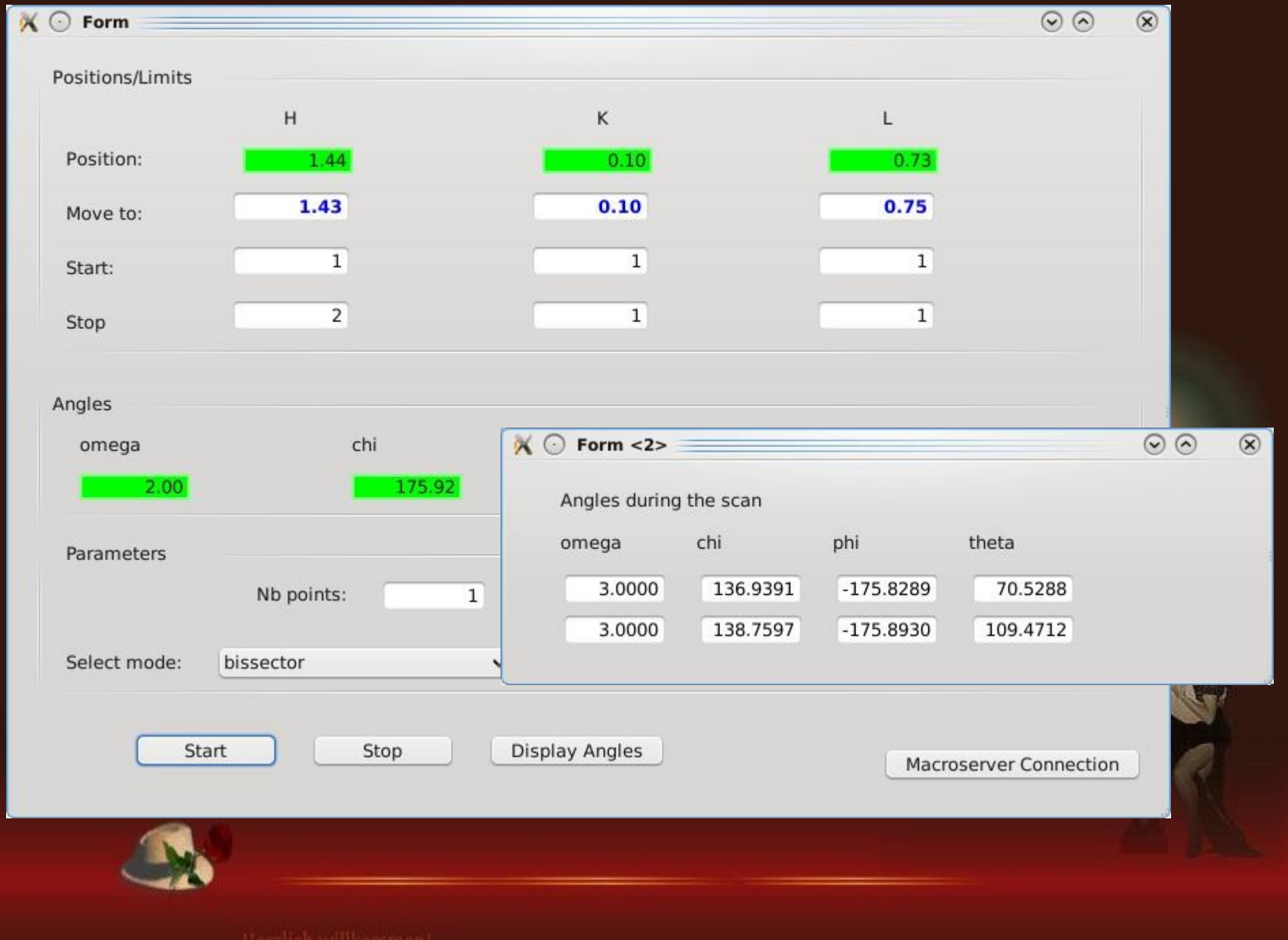
- HKL GUIs:
  - developed based on previous diffractometer GUIs
  - used occasionally at Petra

Example macros:

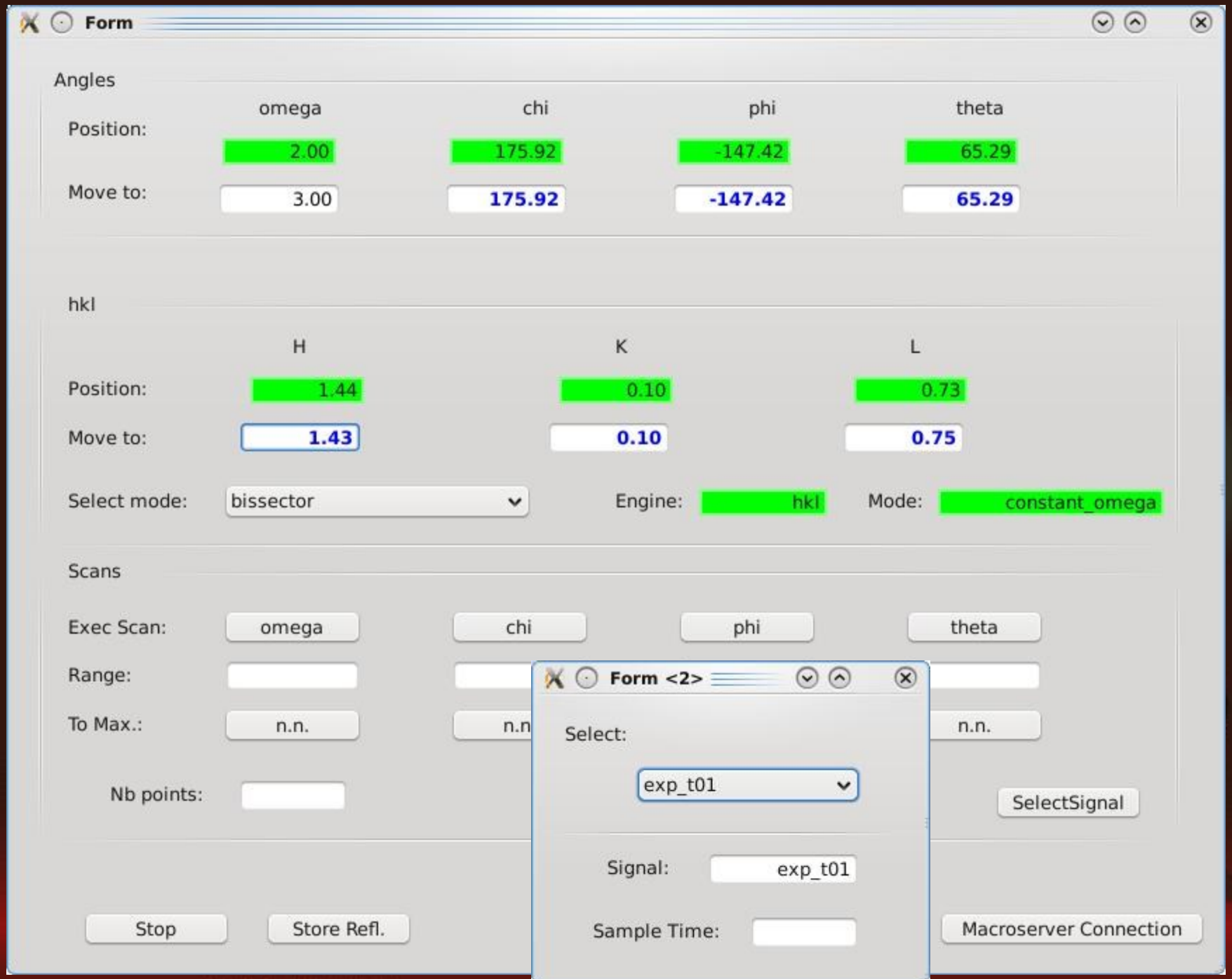
```
tnunez@haso113u: ~ <3>
File  Edit  View  Search  Terminal  Help

Door_hkl_1 [13]: wh

Engine: hkl

Mode: bissector_vertical

H K L =    1.00001   0.00001   0.99999

Azimuth (Psi - calculated) =  73.71852
Wavelength =  1.54000

     Delta       Theta          Chi          Phi          Mu       Gamma
  36.19600    18.09800    -41.05900    78.66200    1.00000    93.84000

Door_hkl_1 [14]: br 0 1 1

Door_hkl_1 [15]: ca 1 0 1
Trajectory 0 (more trajectories by caa H K L)

Azimuth (Psi) =  -118.33989
Wavelength =  1.54000

     Delta       Theta          Chi          Phi          Mu       Gamma
  36.19617    18.09808    -41.05921    78.66152    1.00000    93.83995

Door_hkl_1 [16]: ci 1 18 -41 78.66 93.8 36.19
h 0.998711 k 0.002379 l 1.000756

Door_hkl_1 [17]: hklscan 0 1 1 0 1 1 2 1
```

pa, ubr, caa, or0, or1, setorn, or_swap, setlat, setaz, th2th, hklscan, hscan, luppsi, freeze, affine, …

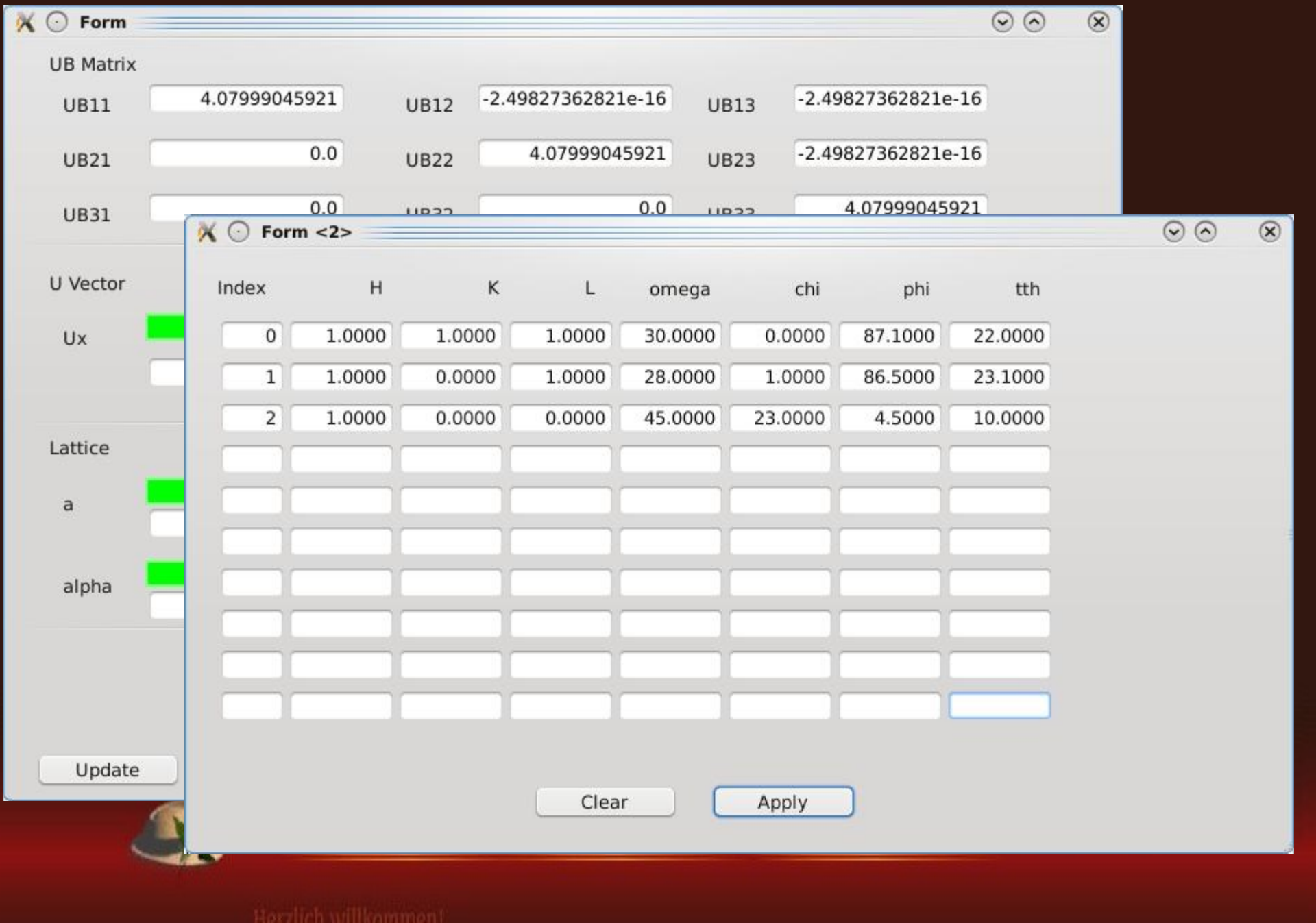

Form
Positions/Limits
H
K
L
Position:
1.44
0.10
0.73
Move to:
1.43
0.10
0.75
Start:
1
1
1
Stop
2
1
1
Angles
omega
chi
phi
theta
2.00
175.92
-147.42
65.29
Parameters
Nb points:
1
Sample time:
1
Select mode:
bissector
Engine:
hkl
Mode:
constant_omega
Start
Stop
Display Angles
Macroserver Connection


Form
Positions/Limits
H
K
L
Position:
1.44
0.10
0.73
Move to:
1.43
0.10
0.75
Start:
1
1
1
Stop
2
1
1
Angles
omega
chi
2.00
175.92
Parameters
Nb points:
1
Select mode:
bissector
Start
Stop
Display Angles
Macroserver Connection
Form <2>
Angles during the scan
omega
chi
phi
theta
3.0000
136.9391
-175.8289
70.5288
3.0000
138.7597
-175.8930
109.4712


Form
Angles
omega
chi
phi
theta
Position:
2.00
175.92
-147.42
65.29
Move to:
3.00
175.92
-147.42
65.29
hkl
H
K
L
Position:
1.44
0.10
0.73
Move to:
1.43
0.10
0.75
Select mode:
bissector
Engine:
hkl
Mode:
constant_omega
Scans
Exec Scan:
omega
chi
phi
theta
Range:
To Max.:
n.n.
n.n.
n.n.
n.n.
Nb points:
SelectSignal
Stop
Store Refl.
Macroserver Connection


Form
Angles
omega
chi
phi
theta
Position:
2.00
175.92
-147.42
65.29
Move to:
3.00
175.92
-147.42
65.29
hkl
H
K
L
Position:
1.44
0.10
0.73
Move to:
1.43
0.10
0.75
Select mode:
bissector
Engine:
hkl
Mode:
constant_omega
Scans
Exec Scan:
omega
chi
phi
theta
Range:
To Max.:
n.n.
n.n
n.n.
Nb points:
SelectSignal
Stop
Store Refl.
Macroserver Connection
Form <2>
Select:
exp_t01
Signal:
exp_t01
Sample Time:


Form
UB Matrix
UB11
4.07999045921
UB12
-2.49827362821e-16
UB13
-2.49827362821e-16
UB21
0.0
UB22
4.07999045921
UB23
-2.49827362821e-16
UB31
0.0
UB32
0.0
UB33
4.07999045921
U Vector
Ux
0.00
0.00
Uy
0.00
0.00
Uz
0.00
0.00
Lattice
a
1.54
1.54
b
1.54
1.54
c
1.54
1.54
alpha
90.00
90.00
beta
90.00
90.00
gamma
90.00
90.00
Update
ComputeU
Reflections List
Edit Reflections


Form
UB Matrix
UB11
4.07999045921
UB12
-2.49827362821e-16
UB13
-2.49827362821e-16
UB21
0.0
UB22
4.07999045921
UB23
-2.49827362821e-16
UB31
0.0
0.0
4.07999045921
U Vector
Ux
Lattice
a
alpha
Update
Form <2>
Index
H
K
L
omega
chi
phi
tth
0 1.0000 1.0000 1.0000 30.0000 0.0000 87.1000 22.0000
1 1.0000 0.0000 1.0000 28.0000 1.0000 86.5000 23.1000
2 1.0000 0.0000 0.0000 45.0000 23.0000 4.5000 10.0000
Clear
Apply

Next Steps

- Introduction of macros and GUIs in repository
- SEP to Candidate and Accepted
- Adapt according to feedback from outside DESY

Thanks to:

- F. Picca
- Alba group (Zibi, Carlos P., …) & Tiago
- S. Francoual and J. Strempfer (Petra Scientists)