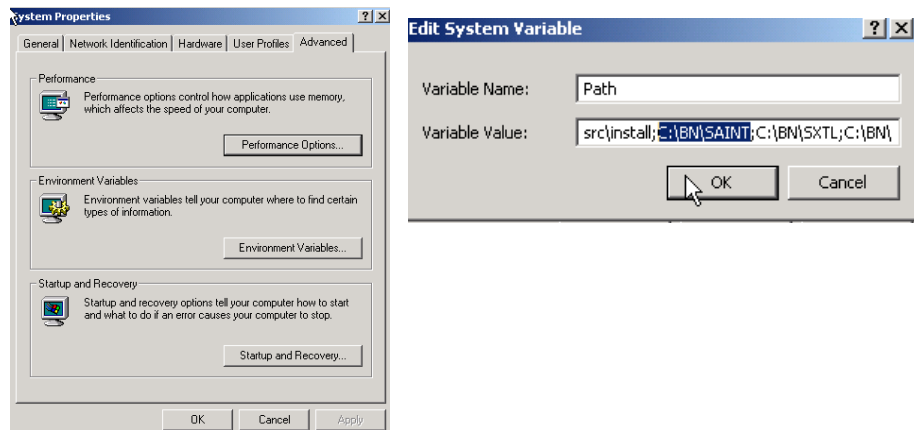


Technical Note 2006-09-21

Apex II data reduction, off-line, off-computer.

If you need to reduce your APEX II data on your computer, you will need to run the latest version of SAINT.

1. Obtain SAINT for the laboratory manager.
2. Copy the SAINT directory to a new directory on your computer
 - a. For example copy the directory to C:\BN\SAINT
3. Rename SAINT.EXE to SAINT_APEX.EXE
4. set the PATH in the Environment Variables



5. Open a command window and navigate to the directory with the frames data
6. Start the data reduction by typing SAINT_APEX

```
Shortcut to CMD.EXE
Microsoft Windows [Version 5.00.2195]
(C) Copyright 1985-2000 Microsoft Corp.

F:\structures>cd fep
F:\structures\Fep>cd apexII
F:\structures\Fep\apexii>cd feph
F:\structures\Fep\apexii\feph>saint_apex_
```

```
Shortcut to CMD.EXE - saint_apex
SAINT+ Integration Engine U7.23A
Copyright (c) 1997-2005 Bruker AXS, Inc. All rights reserved.

MASTER MENU
Command      Description
EXIT,QUIT   End program. Return to operating system
HELP        Display on-line documentation
SYSTEM      Temporarily invoke system command line
INTEGRATE   Compute intensities for a series of frames
FILTER      Selectively modify a reflection file
SORT        Sort reflections according to point group
STATISTICS  Compute tabular summary of reflection file
CONFIGURE   Set up parameters or save/restore a setup
GLOBAL      Re-run a global unit cell refinement

SAINT> configure
```

7. Enter Configure

```

Shortcut to CMD.EXE - saint_apex
Current INI file: saint.ini

[A]Absorption coeff per CM for air 0.0010
[I]Faceplate transmittance at normal incidence 0.9970

[D]Detector type 1
  # Pixels/CM          81.92          CM to detection plane 0.80
  Brass plate spacing 0.254          Readout noise (e-)   14.0
  Electrons per ADU   2.30           Electrons/x-ray photon 15.0
  Base offset / exposure 16          Full scale A/D value 500000

[S]Set detector [D] parameters to defaults
[R]Read new configuration from disk file
[W]Write (save) configuration to a file
[Q]Quit -- return to previous menu

Command: S

Entering -9999 at the following prompt will set all the
detector parameters to -9999, indicating that they should
be retrieved from the frame headers during integration,
or from the .ma file during global cell refinement. This
will work on new data sets, but may cause termination
with an error message in the case of older CCD frames or
.ma files which do not contain the necessary information.

Detector type (0=MW, 1=CCD, 2=APEX CCD, -9999=get from frames): [I] -9999

```

8. Enter S and -9999 for detector type

```

Shortcut to CMD.EXE - saint_apex

[T]Title: Fe CpPPh2
[I]Input frame 1: ylid0.001
[M]Or. matrix filename: ylid0.p4p
[C]Spatial cal filename: $P4P
[N]#Frames: 9999
[N]Timeout(sec) 0.00          [Z]Beam monitor N      [E]Exposure 0.00
[X]Monochr 2Th 12.17         Roll 0.00             [B]Batch# 1           [K]Crystal 1

[R]Output refl filename: ylid0.raw
[F]Snapshot freq 0          [+A]Append N          [U]Resolution 0.900   [#]I/sigma -3.00
[U]Verbosity 1              Plotfiles N           [J]Sample Map 1
[P]PointGp mmm              Lattice 0

[S]Spot size:                X(deg) 1.500           Y(deg) 1.500          Z(deg) 0.600
[H]Strong thresh (I/sigma) 10.0 [O]Wide frames N     [L]LS profile fit N

[V]Local ref: Freq 40       CrySys 0           Param mask 512        [-]Wt Meth 2
[G]Global ref: Enab Y       CrySys 0           Param mask 0          [X]RLU Err 0.0250

[A]Advanced options...      [D]Enter new default base filename
[I]Begin integration        [Q]Quit -- return to previous menu

Command: I

Name of first frame ? [ylid0.001] test_01_0001.sfrm,test_02_0001.sfrm,test_03_0001.sfrm,test_04_0001.sfrm

```

9. Quit – return to previous menu and type I. Enter all of the frame sets you want to reduce, be sure you enter the entire name and separate them by commas.

```

Shortcut to CMD.EXE - saint_apex
[Title: Fe CpPPh2
[Input frame 1: test_01_0001.sfrm,test_02_0001.sfrm,test_03_0001.sfrm,test_0
[M]Or. matrix filename: ylid0.p4p
[C]Spatial cal filename: $P4P
[N]#Frames: 9999
[W]Timeout(sec) 0.00 [Z]Beam monitor N [E]Exposure 0.00
[2]Monochr 2Th 12.17 Roll 0.00 [B]Batch# 1 [K]Crystal 1

[R]Output refl filename: ylid0.raw
[F]Snapshot freq 0 [+A]ppend N [U]Resolution 0.900 [#]I/sigma -3.00
[U]Verbosity 1 Plotfiles N [J]Sample Map 1
[P]PointGp mmm Lattice 0

[S]Spot size: X(deg) 1.500 Y(deg) 1.500 Z(deg) 0.600
[H]Strong thresh (I/sigma) 10.0 [O]Wide frames N [L]LS profile fit N

[Y]Local ref: Freq 40 CrySys 0 Param mask 512 [-]Wt Meth 2
[G]Global ref: Enab Y CrySys 0 Param mask 0 [X]RLU Err 0.0250

[A]Advanced options... [D]Enter new default base filename
[!]Begin integration [Q]Quit -- return to previous menu

Command: m
Orientation matrix (.spin, .p4p, or ._pr) filename ? [ylid0.p4p] test.p4p,test.p4p,test.p4p,test.p4p_

```

10. type M and enter the P4P file that you created in APEX. Enter the name once for each frame set, separated by commas.

11. Make sure the special cal filename is \$P4P

```

Shortcut to CMD.EXE - saint_apex
[Title: Fe CpPPh2
[Input frame 1: test_01_0001.sfrm,test_02_0001.sfrm,test_03_0001.sfrm,test_0
[M]Or. matrix filename: test.p4p,test.p4p,test.p4p,test.p4p
[C]Spatial cal filename: $P4P
[N]#Frames: 9999
[W]Timeout(sec) 0.00 [Z]Beam monitor N [E]Exposure 0.00
[2]Monochr 2Th 12.17 Roll 0.00 [B]Batch# 1 [K]Crystal 1

[R]Output refl filename: ylid0.raw
[F]Snapshot freq 0 [+A]ppend N [U]Resolution 0.900 [#]I/sigma -3.00
[U]Verbosity 1 Plotfiles N [J]Sample Map 1
[P]PointGp mmm Lattice 0

[S]Spot size: X(deg) 1.500 Y(deg) 1.500 Z(deg) 0.600
[H]Strong thresh (I/sigma) 10.0 [O]Wide frames N [L]LS profile fit N

[Y]Local ref: Freq 40 CrySys 0 Param mask 512 [-]Wt Meth 2
[G]Global ref: Enab Y CrySys 0 Param mask 0 [X]RLU Err 0.0250

[A]Advanced options... [D]Enter new default base filename
[!]Begin integration [Q]Quit -- return to previous menu

Command: R
Output reflection file pathname ? [ylid0.raw] t1.raw,t2.raw,t3.raw,t4.raw_

```

12. Enter the raw data file names, one for each frame set. I have named them t1 to t4.raw

```

C:\> Shortcut to CMD.EXE - saint_apex
[Title: Fe CpPPh2
[Input frame 1: test_01_0001.sfrm,test_02_0001.sfrm,test_03_0001.sfrm,test_0
[M]Or. matrix filename: test.p4p,test.p4p,test.p4p,test.p4p
[C]Spatial cal filename: $P4P
[N]#Frames: 9999
[W]Timeout(sec) 0.00 [Z]Beam monitor N [E]Exposure 0.00
[M]Monochr 2Th 12.17 Roll 0.00 [B]Batch# 1 [K]Crystal 1

[R]Output refl filename: t1.raw,t2.raw,t3.raw,t4.raw
[F]Snapshot freq 0 [+A]Append N [U]Resolution 0.900 [#]I/sigma -3.00
[U]Verbosity 1 Plotfiles N [J]Sample Map 1
[P]PointGp -1 Lattice 0

[S]Spot size: X(deg) 1.500 Y(deg) 1.500 Z(deg) 0.600
[H]Strong thresh (I/sigma) 10.0 [O]Wide frames N [L]LS profile fit N

[Y]Local ref: Freq 40 CrySys 0 Param mask 512 [-]Wt Meth 2
[G]Global ref: Enab Y CrySys 0 Param mask 0 [X]RLU Err 0.0250

[A]Advanced options... [D]Enter new default base filename
[!]Begin integration [Q]Quit -- return to previous menu

Command: u
Best resolution (A) to include in output ? [0.900] .5_

```

- Change the best resolution to a lower value say .5 and the spot size to 1.5 1.5 1.0. Type L to start the LS profile fit. .

```

C:\> Shortcut to CMD.EXE - saint_apex
[Title: Fe CpPPh2
[Input frame 1: test_01_0001.sfrm,test_02_0001.sfrm,test_03_0001.sfrm,test_0
[M]Or. matrix filename: test.p4p,test.p4p,test.p4p,test.p4p
[C]Spatial cal filename: $P4P
[N]#Frames: 9999
[W]Timeout(sec) 0.00 [Z]Beam monitor N [E]Exposure 0.00
[M]Monochr 2Th 12.17 Roll 0.00 [B]Batch# 1 [K]Crystal 1

[R]Output refl filename: t1.raw,t2.raw,t3.raw,t4.raw
[F]Snapshot freq 0 [+A]Append N [U]Resolution 0.500 [#]I/sigma -3.00
[U]Verbosity 1 Plotfiles N [J]Sample Map 1
[P]PointGp -1 Lattice 0

[S]Spot size: X(deg) 1.500 Y(deg) 1.500 Z(deg) 1.000
[H]Strong thresh (I/sigma) 10.0 [O]Wide frames N [L]LS profile fit Y

[Y]Local ref: Freq 40 CrySys 0 Param mask 512 [-]Wt Meth 2
[G]Global ref: Enab Y CrySys 0 Param mask 0 [X]RLU Err 0.0250

[A]Advanced options... [D]Enter new default base filename
[!]Begin integration [Q]Quit -- return to previous menu

Command: !

```

- Type ! (bang) to start the integration.
- Saint will start and reduce the data.
- When finished exit the program and save the SAINT.INI.
- When complete all of the files generated will be in the same directory as the data frames. Move the new files to a new directory and run sadabs.
- Complete the structure in the normal fashion.