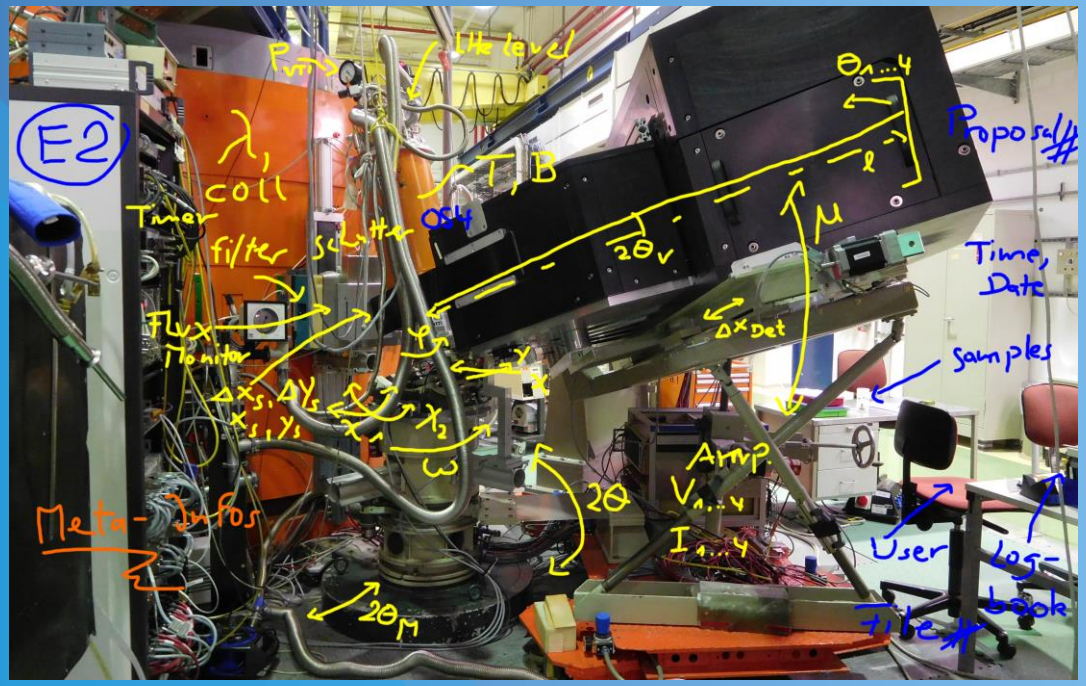
NeXus at the Flat-Cone Diffractormeter E2

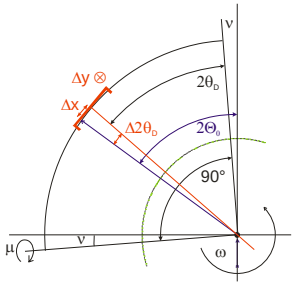
Data and Workflow Concepts



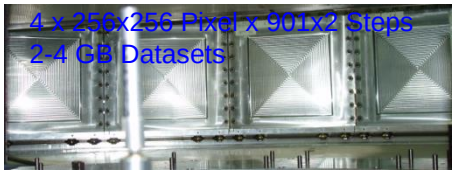
Jens-Uwe Hoffmann, Quantum Phenomena in Novel Materials (EM-IQM)

Agenda

Instrument Control
CARESS



Raw Detector Datasets



Root (Cern) Histogram

Meta Information

NeXus
HDF5
PNI-HDRI Standard

Parameter, axes information &
h,k,l,E, T,H, etc.

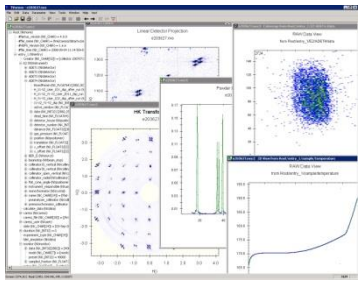
converting and pre-analysis → User Format

- Flat-Cone Diffractometer
- Data Sources
- Data Flow
- NeXus
- Automatic Analysis
- Scientific Workflow
- Creating new Meta-Data

Nexus Server

Findable
Accessible
Interoperable
Reusable

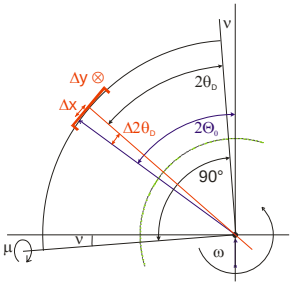
Instrument near or general software



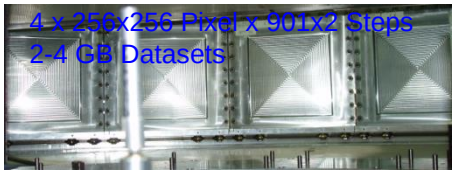
TV*neXus*
- Visualization
- Transformation
- Corrections
- Data transfer to analyze software
- Modeling

Agenda

Instrument Control
CARESS



Raw Detector Datasets



Root (Cern) Histogram

Meta Information

NeXus
HDF5
PNI-HDRI Standard

Parameter, axes information &
h,k,l,E, T,H, etc.

converting and pre-analysis → User Format

XML-Meta-Info (& Caress)

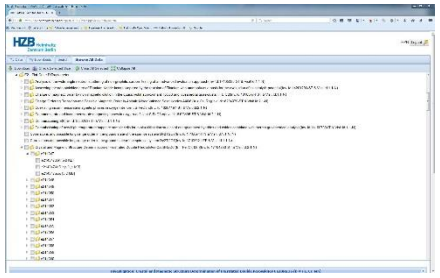
ICAT

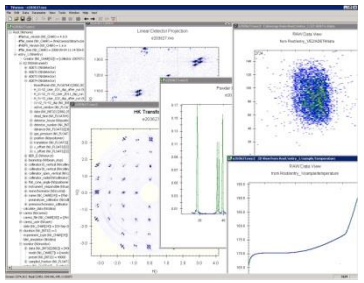
Archiving and
Documentation

Nexus
Server

Instrument near or general software

TOPCAT





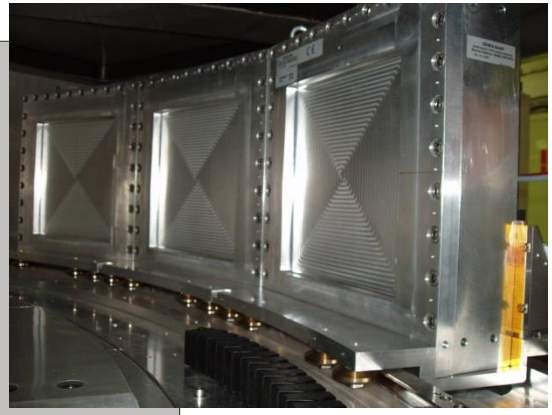
TV*neXus*
- Visualization
- Transformation
- Corrections
- Data transfer to analyze software
- Modeling

Findable
Accessible
Interoperable
Reusable

The Neutron Flat-Cone Diffractometer E2 (2007)

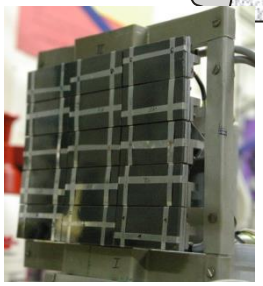
Uncompressed low structured data sets up to 4 GB

Collimator Changer (15‘/30‘/60‘ open) $(dq/q)_{best}<10^{-2}$



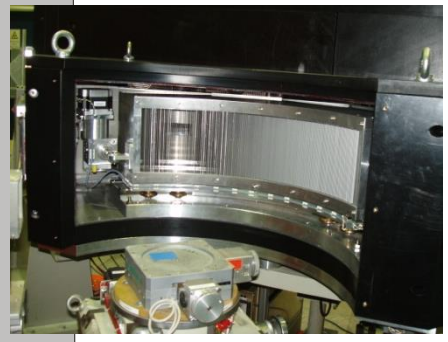
Individual positionable with „waggons“

R 1



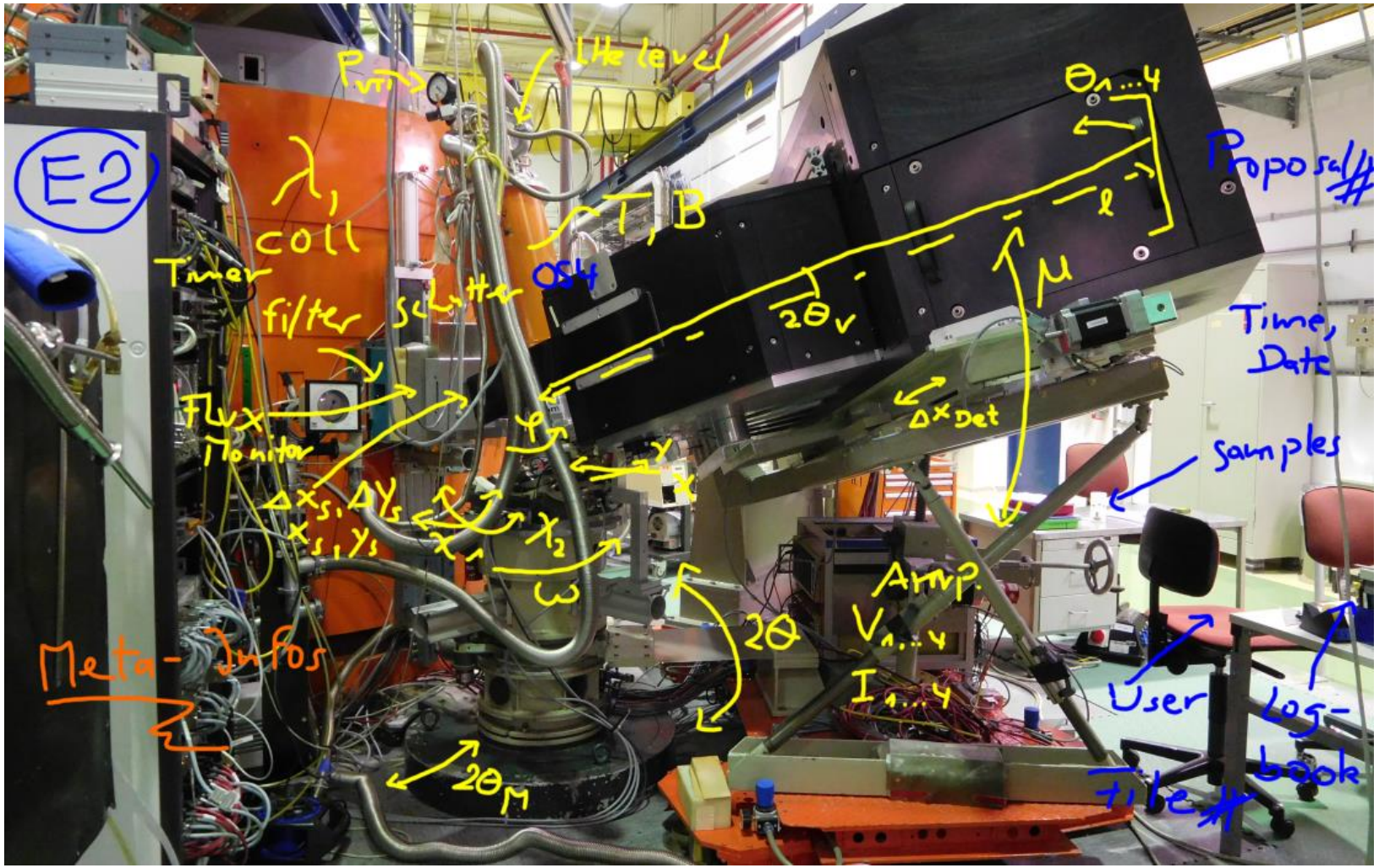
3 monochromators on changing device
λ= 0.90 Å, 1.21 Å and 2.39 Å
q_{max}(Cu)=10.8 Å^{-1}

Four 2D-Detectors
$3^o < 2\theta_h < 110^o$
$-2.5^o < 2\theta_v < +7.5^o$



Radial Collimator

Meta Data


E2
λ
coll
Timer
filter
Flux
Monitor
T, B
OSA
2θv
θ1...4
Proposal #
Time, Date
Δx Det
samples
Amp.
V1...4
I1...4
2θ
2θM
Meta-Infos
User
Log-book
file #

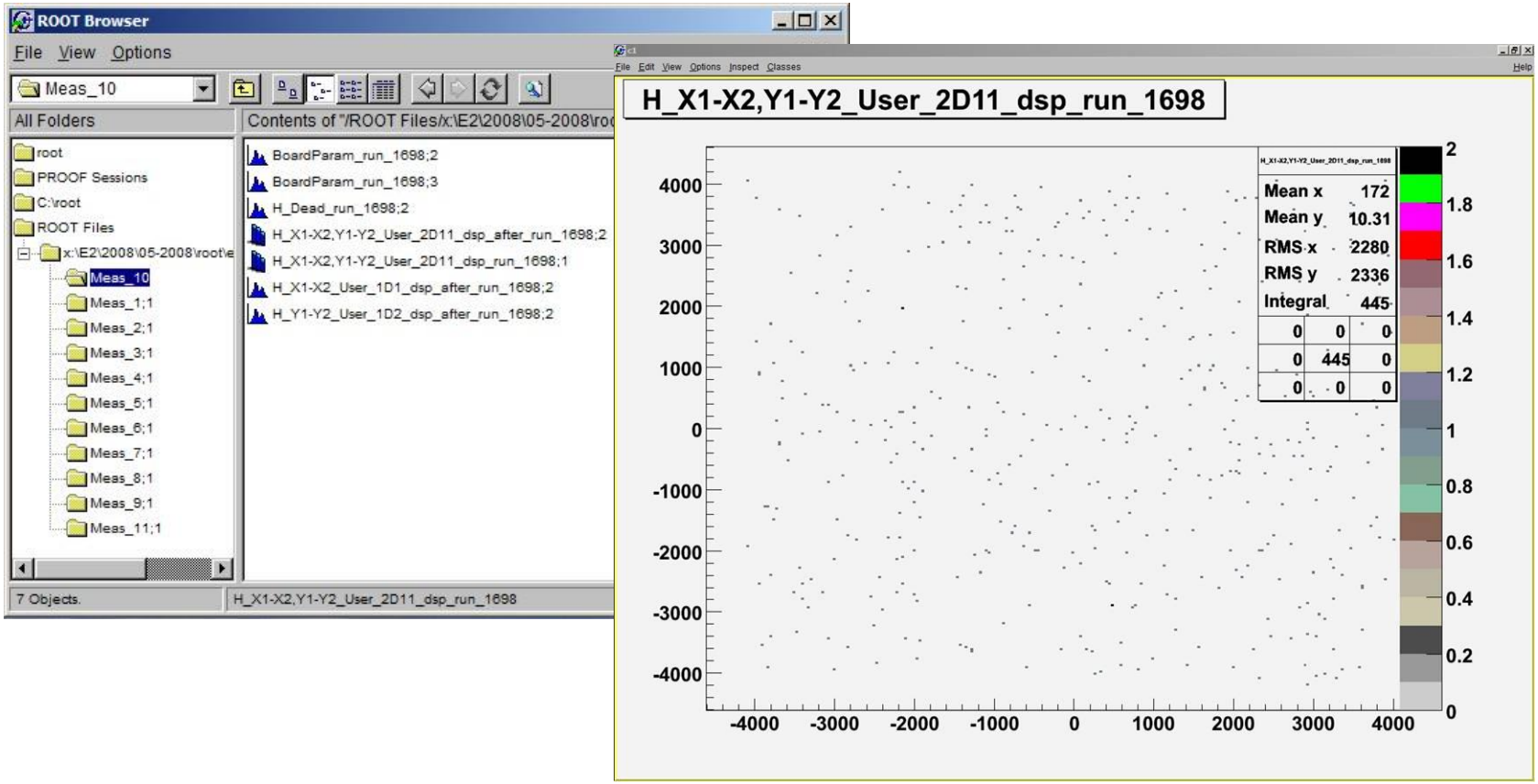
CARESS binary logging file

SYS$SYSDEVICE:[CARESS.DATA]E236019.DAT;1 …
NUMOR 36019
EXPTYPE E2,A2,LDET,FLAT
USN JUH
BLS OMGS=-8.15000E+01, 2.31000E+02 TTHS=-2.00000E+02, 2.00000E+02 PHIS=-2.00000E+02, 2.00000E+02 … SOF …. TOL …
WAV 0.00000E+00
MM1 TIM1= 10
SL1 TTHS LDET MON
SAM SAMPLE … TITLE TESTMESSUNG
READ TTHS=-4.99500E+00 PHIS= 9.00010E+01 OMGS= 2.49939E-02 T_REG= 1.02900E+02 T_SAM=-1.00000E+03 …
SGEN1 STEP= 11 COLL15T= 3.33000E+02, 3.63000E+02
DATE 15-JAN-03 … TIME 16:37:14

SETVALUES …. COLL15T 333.0000
MASTER1VALUES … MM1 … TIM1 10
LDET …. W1 … 1/ 74.81 0 0 0 0 0 0 0 0 0 0 ..
MON 121
SETVALUES … COLL15T 336.0000

MASTER1VALUES … MM1 … TIM1 10
LDET …. W1 … 1/ 74.81 0 0 0 0 0 0 0 0 0 0 ..
MON 121
SETVALUES … COLL15T 339.0000
…
DATE 15-JAN-03… TIME 16:39:51

Data Storage – Root (from root.Cern.ch)



Semi-static Information

Hardware Moduls

```
;-------------------------------------------------------------------
; serial port (Nhardware_modules_e2.datetCom ?11/?13 ethernet se
;name   kind    host            port#   unit#   baud    data
;                ip-address                      rate    bits
;NETCOM1 60      192.168.1.11    1       0       9600    7
;NETCOM2 60      192.168.1.11    2       1       9600    7
;NETCOM3 60      192.168.1.10    1       2       9600    7
;NETCOM4 60      192.168.1.10    2       3       9600    7
#endif

; E2 pressure (2015-11-25)
;DRUCK  500     Druck

#if MAGF
;Oxford IPS120chi2=0 chi1=0
;name   kind    ieee    unit#   gpibaddr    non-persistant (1)
MAGF    44      2       0       25          0
#endif

; ST222 motor controller
;  motor type:   "CopleyStepnet" for ST222-MOT and ST224-MOT
;  encoder type: "BeckhoffKL5001" for SSI inputs on ST222-ENC
; name          kind    CORBA reference to CPU
MONOC           500     corbaname::dist222dh0829#st222.caress_ob
OMGM            500     corbaname::dist222dh0829#st222.caress_ob
M1_FOC1         500     corbaname::diminil#st222.caress_object
M1_FOC2         500     corbaname::diminil#st222.caress_object
MONTR           500     corbaname::dist222dh0829#st222.caress_ob
MONTI           500     corbaname::dist222dh0829#st222.caress_ob
;TTHM           500     corbaname::dist222dh0829#st222.caress_ob
COLL15          500     corbaname::diminil#st222.caress_object
COLL30          500     corbaname::diminil#st222.caress_object
COLL15T         500     corbaname::diminil#st222.caress_object
COLL30T         500     corbaname::diminil#st222.caress_object

;name   kind    bus             ?       motor1  motor2
;                3=ST180         unit#
;                6=COMBO         ignore
COLL    40      6               0       COLL15  COLL30

TTHS            500     corbaname::diminil#st222.caress_object
; factor (Motor) =144000 (Motor) / 8192 (Encoder) * divider (Enc
; alte Wert 40000
; neue Wert 38000
TTH1            500     corbaname::diminil#st222.caress_object
TTH2            500     corbaname::diminil#st222.caress_object
```

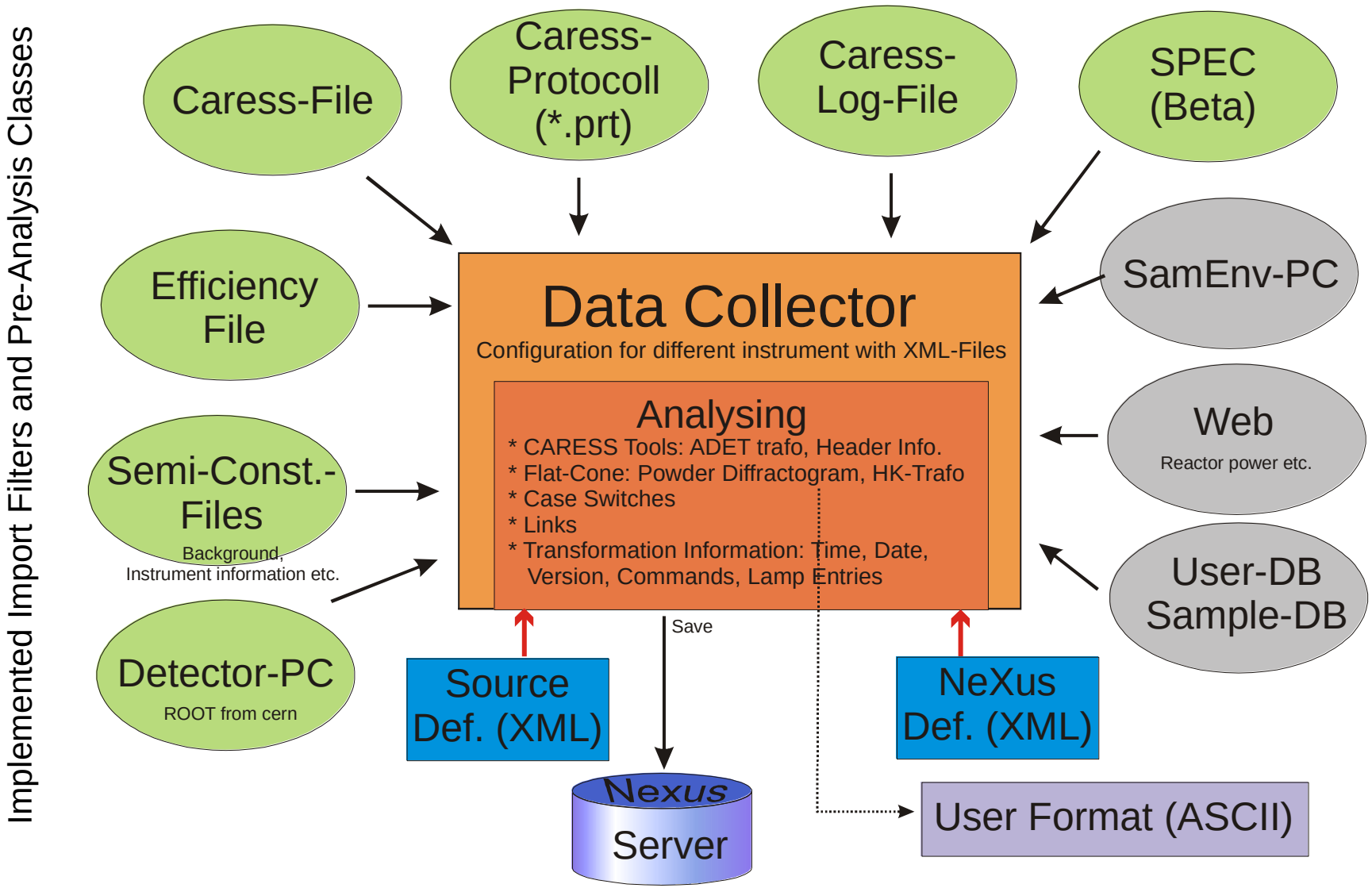
Corba Devies

```
[MONOC]
; Motor: 4000 Mikroschritte/Grad
; Encoder: 4096 Mikroschritte/Grad
; Maximalbeschleunigung * 10 Schritte/sec^2)
;motion_motor_acceleration = 500
; Maximalgeschwindigkeit * 0.1 Mikroschritte/sec
;motion_motor_maximum speed = 60000
; Hold current *0.01A
;motion_motor_hold current = 50
motion_motor_currentoff = true
motion_usefloat = true
motion_autodelete = false
start = never, async
;stop = never, async
stop = premaster, async
stopkinds=11,12,0x8000000B,0x8000000C
read = auto, async
;motion_display = 30
;motion_displayformat = %0.3f

[OMGM]
; Motor: 4000 Mikroschritte/Grad
; Encoder: 4096 Mikroschritte/Grad
; Maximalbeschleunigung * 10 Schritte/sec^2)
; motion_motor_acceleration = 500
; Maximalgeschwindigkeit * 0.1 Mikroschritte/sec
;motion_motor_maximum speed = 30000
motion_usefloat = true
motion_autodelete = false
start = never, async
;stop = never, async
stop = premaster, async
stopkinds=11,12,0x8000000B,0x8000000C
read = auto, async
;motion_display = 29
;motion_displayformat = %0.3f

[MONTR]
; Motor: 4000 Mikroschritte/Grad
; Encoder: 4096 Mikroschritte/Grad
; Maximalbeschleunigung * 10 Schritte/sec^2)
;motion_motor_acceleration = 500
; Maximalgeschwindigkeit * 0.1 Mikroschritte/sec
;motion_motor_maximum speed = 7000
motion_usefloat = true
motion_autodelete = false
```

Efficiency File

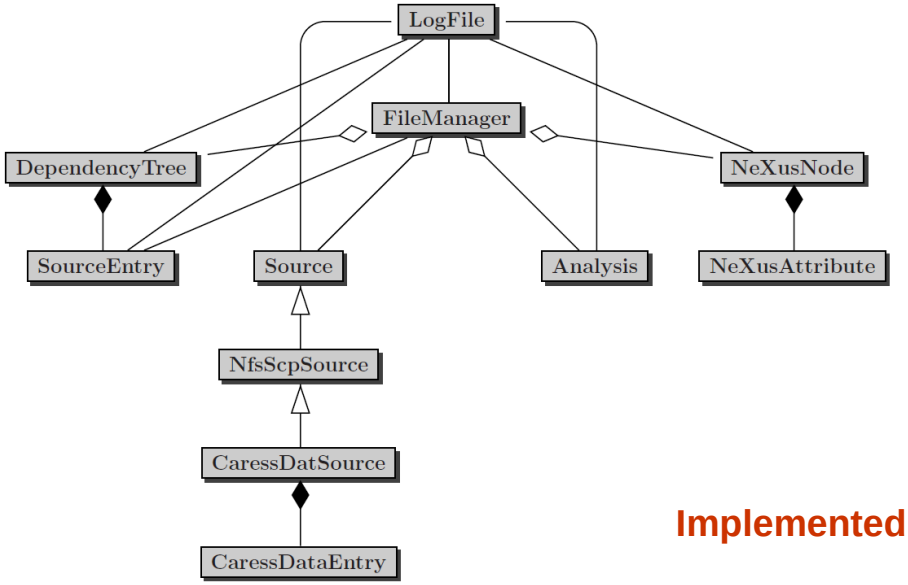
```
                <LINE83>
# # # # # # # # # #
# # # # # # # # # #
1.27325 1.19228 1.20691 1.20192 1.17365 1.19039 1.17028
1.19682 1.16935 1.15106 1.16146 1.1859 1.18339 1.18851
1.19421 1.17067 1.14649 1.19607 1.17372 1.18461 1.21036
1.16556 1.16089 1.17494 1.18573 1.16676 1.12795 1.14706
1.1412 1.13301 1.14801 1.1624 1.16384 1.15992 1.18412 1
1.1987 1.17608 1.18056 1.19431 1.18521 1.16237 1.17783
1.17809 1.17437 1.17815 1.17084 1.18512 1.19459 1.18444
1.14063 1.14362 1.12112 1.13706 1.14476 1.13874 1.16158
1.13925 1.16319 1.18157 1.16388 1.19607 1.18044 1.16138
1.16571 1.1771 1.19478 1.19676 1.18908 1.18525 1.13537
1.17539 1.20742 1.17772 1.20988 1.21853 1.17659 1.2107
1.16845 1.17215 1.21557 1.18815 1.23866 1.20114 1.19335
1.20598 1.14869 1.16552 1.19649 1.18164 1.16217 1.14311
1.16872 1.17055 1.17149 1.18972 1.18449 1.19457 1.18813
1.14531 1.15145 1.14697 1.16296 1.16289 1.13543 1.1505
1.1913 1.16956 1.16932 1.16252 1.17176 1.13209 1.1604 1
1.18849 1.1537 1.17867 1.17244 1.18134 1.18348 1.14869
1.16453 1.13876 1.13517 1.14156 1.18344 1.18248 1.1514
1.1447 1.08453 1.18791 1.1884 1.20514 1.15902 1.11611 1
1.15564 1.18044 1.18679 1.15833 1.14789 1.1717 1.16078
1.18737 1.17732 1.18135 1.16358 1.1874 1.16063 1.16632
1.19361 1.18827 1.1633 1.12931 1.19352 1.19812 1.20706
# # # # # # # # # #
# # # # # #
</LINE83>
                <LINE84>
# # # # # # # # # #
# # # # # # # # # #
1.02702 1.01071 1.0156 1.01389 0.986128 0.991616 0.9988
0.973427 0.968885 0.981554 0.981876 0.966616 0.9804 0.9
1.00354 0.980168 0.988951 0.98141 0.980429 0.970134 0.9
0.957278 0.96839 0.970084 0.995922 0.961236 0.969742 0.
0.942617 0.95453 0.937845 0.968585 0.939757 0.960962 0.
0.991157 0.980165 0.961825 0.989494 0.989182 0.986679 0
0.969864 0.970075 0.978616 0.984076 0.969848 0.965152 0
0.969929 0.930806 0.939937 0.94872 0.94348 0.934969 0.9
0.957067 0.954751 0.980569 0.979239 0.971209 0.976504 0
0.99009 0.982664 0.972739 0.999728 0.982918 0.968223 0.
1.03126 0.997263 1.03723 1.03435 0.976944 1.01088 1.012
0.996408 0.975268 0.992804 0.995335 1.00042 0.99799 0.9
0.99347 0.935062 0.975168 0.981201 0.956706 0.955117 0.
0.942742 0.941241 0.970204 0.953722 0.954605 0.939865 0
0.924232 0.920147 0.902555 0.900636 0.919243 0.928901 0
0.943247 0.959313 0.943051 0.940905 0.923259 0.922508 0
```

Data Collector

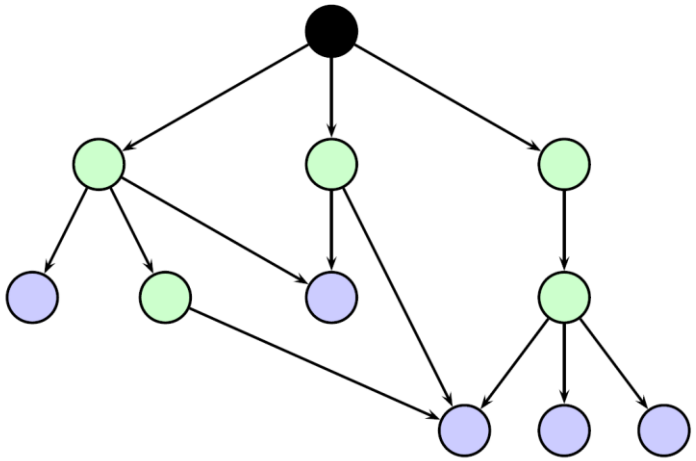


Design of the data collector software

Class schema of data collector
Object oriented concept



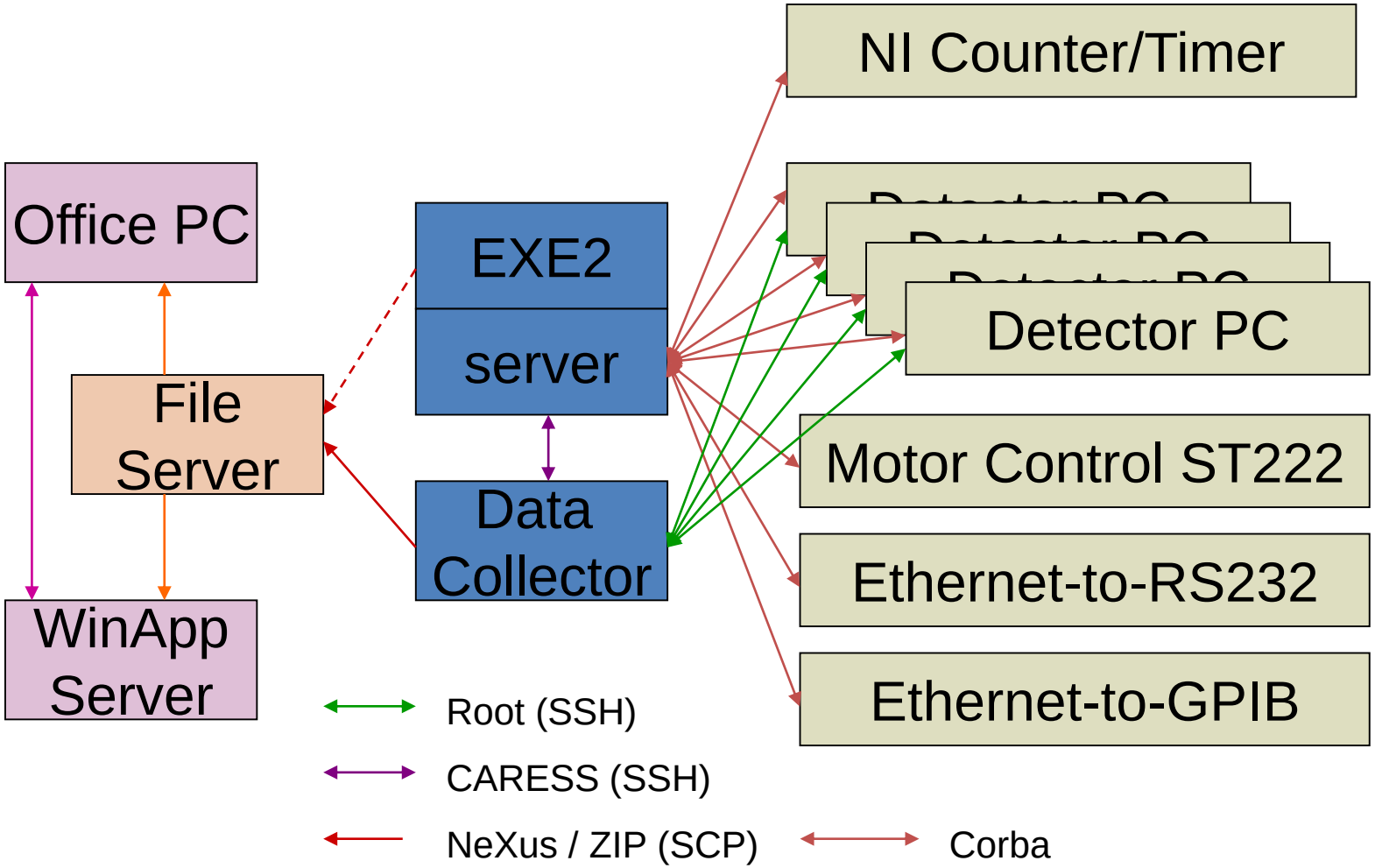
Multi-trees for thread management
Order of executing.



Implemented for LINUX

Diploma thesis: Jörg Gasse, „Konzeptionierung und Erstellung einer Software zur Serialisierung und automatisierten Analyse von komplexen Daten aus unterschiedlichen Quellen“, 2006

Communication Structure



Source-File

```
<?xml version="1.0" encoding="utf-8" ?>
<SourceConfig>
  <Options>
    <LogFile enabled="true" append="false" />
    <ScreenLog enabled="true" />
    <Threads>
      <General>10</General>
      <DataAquisition>1</DataAquisition>
      <DataTransfer>1</DataTransfer>
      <Analyses>5</Analyses>
    </Threads>
    <NeXusFile>/hmi/caress/data/data/e2.nxs</NeXusFile>
    <TempDirectory>/hmi/caress/data</TempDirectory>
  </Options>
  <Sources>
    <Source medium="nfs" type="$CaressDat" name="1">
      <Dependencies>
        <Dependency type="command line">
          <Parameter number="0" wildcard="*" />
        </Dependency>
      </Dependencies>
      <Path>/hmi/caress/data/caress/*.dat</Path>
    </Source>
 </Sources>
</SourceConfig>
```

Implemented Sources

type	subtype	medium	Beschreibung
$CaressDat		nfs	Liest Caress File ein
	$Header		Liest ganzen Zweig von CARESS ein
$DetectorPC		nfs	Beschafft sich Root Daten vom Detector PC und liest diese ein
$ADetAna		nexus	Analysiert ADET Caress Daten und formt diese in ein Array um
$InsertFile		nfs	Fügt ein ASCII File ein
$Link			Ermöglicht Link zu internen Daten; nicht in Sourcedatei
$FlatCone		nexus	Berechnet Pulver-Diffraktogramm und HK-Trafo
	PowderData		Pulver-Daten normiert
	PowderRaw		Pulver-Daten summiert
	PowderMon		Monitorwerte summiert aus Pulver-Daten
	HKtrafoData		Normierte HK-Transforamtion
	HKtrafoRaw		Summierte HK-Daten
	HKtrafoMon		Monitorewerte summiert aus HK-Trafo
	Monitor		Refernezmonitor für Normierung
	HAxis		H-Achsenwerte
	KAxis		K-Achsenwerte
	PowderAxis		ZweiTheta-Werte
	HtrafoError		Sigma-Matrix für HK-Trafo
	PowderError		Sigma-Liste für Pulver-Daten

NeXus configuration file (XML DTD)

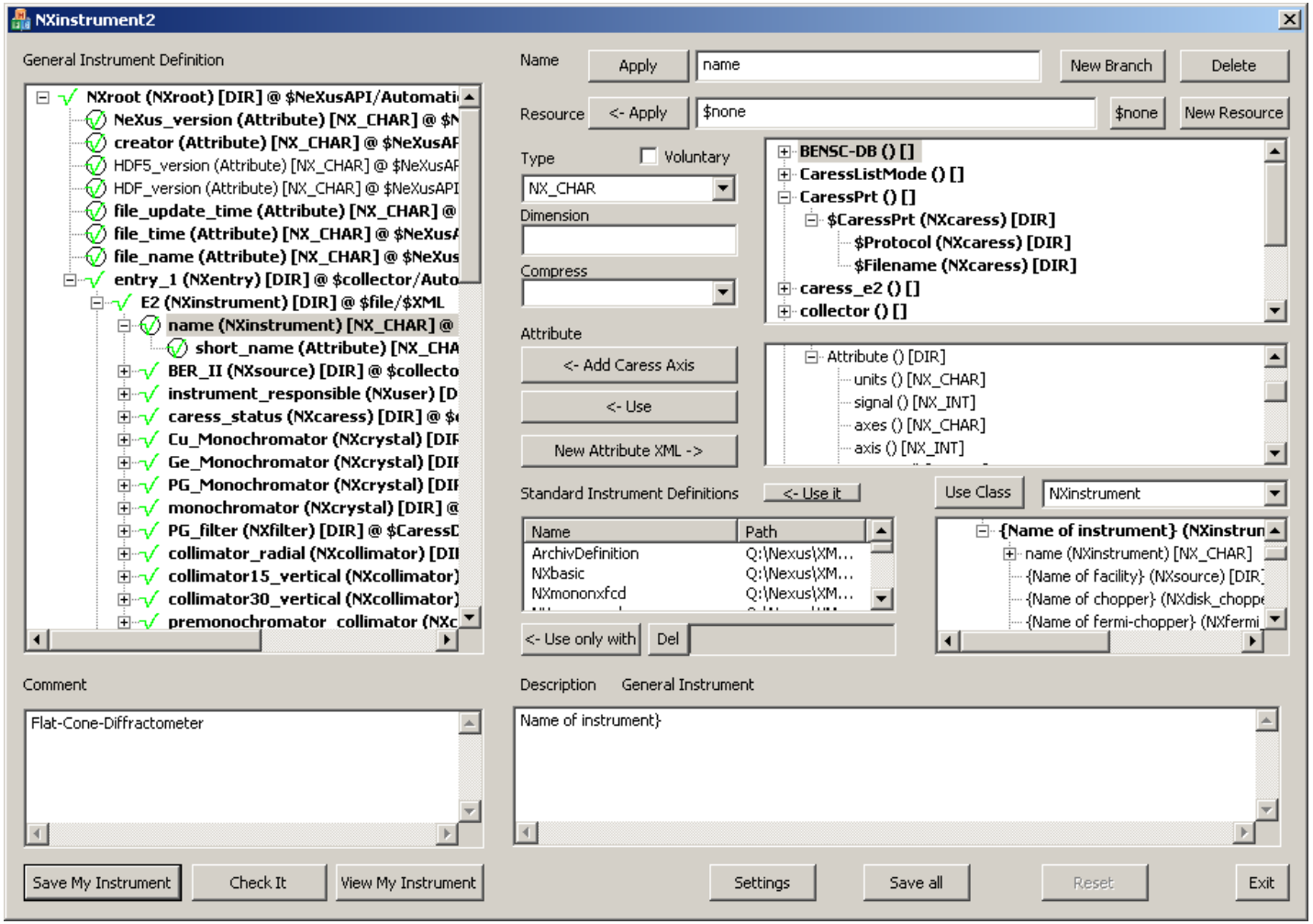
```
<NXbeam nameDef="beam" sourceDef="$collector/Automatic">
      {Details of beam incident on sample - used to calculate sample/beam interaction point}
     <distance typeDef="NX_FLOAT" sourceDef="$none" commentDef="3"
            units = "m" units.typeDef = "NX_CHAR" units.sourceDef = $none">
                  {Distance from sample}
    </distance>
    <final_wavelength typeDef="NX_FLOAT" sourceDef="$CaressDat/WAV"
            units = "angstrom" units.typeDef = "NX_CHAR" units.sourceDef = "$none">
                {Wavelength on leaving beamline component}
    </final_wavelength>
    <monochromator typeDef="NX_FLOAT" sourceDef="$Link/entry_1/E2/monochromator">
          {}
    </monochromator>
</NXbeam>
```

A complex real experiment

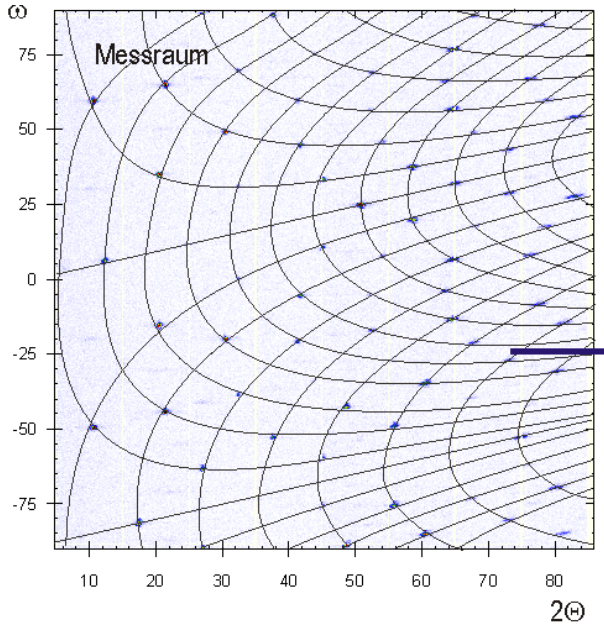
nxdl2_e2.xml

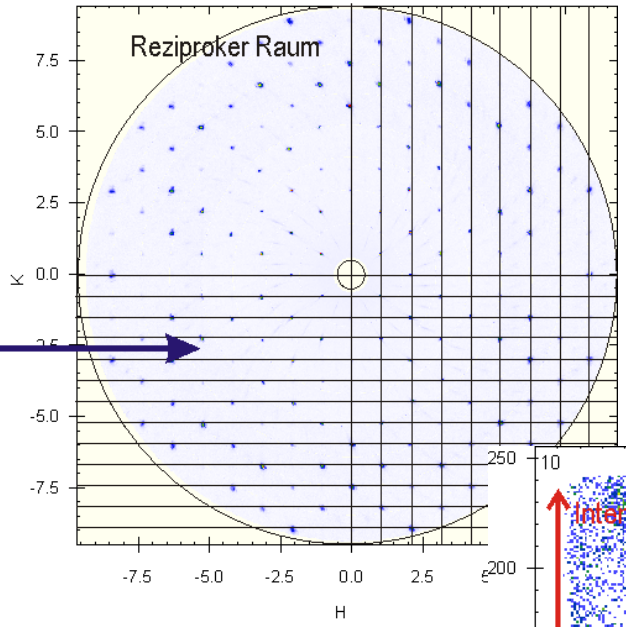
```
<group name="NXroot" type="NXroot" source="$NeXusAPI/Automatic">
  <attribute name="creator" type="NX_CHAR" source="$collector/MyName"> </attribute>
  <attribute name="file_name" type="NX_CHAR" source="$NeXusAPI/Automatic"> </attribute>
  <attribute name="file_time" type="NX_CHAR" source="$NeXusAPI/Automatic"> </attribute>
  <attribute name="file_update_time" type="NX_CHAR" source="$NeXusAPI/Automatic"> </attribute>
  <attribute name="HDF5_version" type="NX_CHAR" source="$NeXusAPI/Automatic"> </attribute>
  <attribute name="HDF_version" type="NX_CHAR" source="$NeXusAPI/Automatic"> </attribute>
  <attribute name="NeXus_version" type="NX_CHAR" source="$NeXusAPI/Automatic"> </attribute>
  <group name="entry_1" type="NXentry" source="$collector/Automatic" compress="NX_COMP_NONE">
    <doc>
    Basic dataset entry
    </doc>
    <group name="caress" type="CARdirectory" source="$collector/Automatic">...
    <group name="powder_diagram" type="NXdata" source="$NeXusAPI/Automatic">
      <field name="data" type="NX_FLOAT64" source="$FlatCone/PowderData" compress="NX_COMP_LZW">
        <doc>
        Data values
        </doc>
      </field>
      <field name="errors" type="NX_FLOAT64" source="$FlatCone/PowderError" compress="NX_COMP_LZW">
      </field>
      <field name="monitor_sum" type="NX_FLOAT64" source="$FlatCone/PowderMon" compress="NX_COMP_LZW">
      </field>
      <field name="polar_angle" type="NX_FLOAT64" source="$FlatCone/PowderAxis">
      </field>
      <field name="referenz_monitor" type="NX_FLOAT64" source="$FlatCone/Monitor" compress="NX_COMP_LZW">
      </field>
      <field name="sum_raw_data" type="NX_FLOAT64" source="$FlatCone/PowderRaw" compress="NX_COMP_LZW">
      </field>
      <field name="x" type="NX_FLOAT64" source="$FlatCone/PowderAxis">
        <doc>
            This is an array holding the values to use for the x-axis of    data.  The units must be appropriate for the measurement.
        </doc>
      </field>
    </group>
    <group name="reciprocal_space" type="NXdata" source="$NeXusAPI/Automatic">...
    <field name="caress_file" type="NX_CHAR" source="$CaressDat/DAT">...
    <field name="end_time" type="ISO8601" source="$CaressDat/$ISO8601/stop">...
    <field name="entry_identifier" type="NX_CHAR" source="$CaressDat/DAT">...
    <field name="experiment_type" type="NX_CHAR" source="$CaressDat/EXPTYPE">...
```

Configuration tool (Windows only)



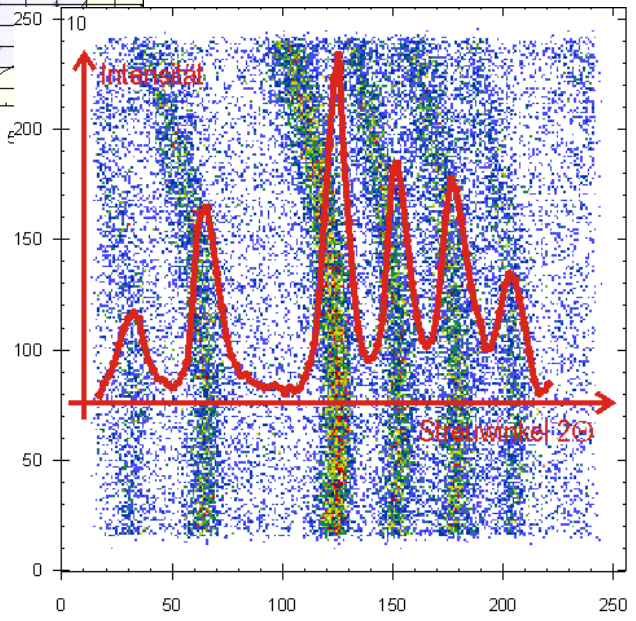
Data Transformations





Single Crystal

Powder



Program Collector

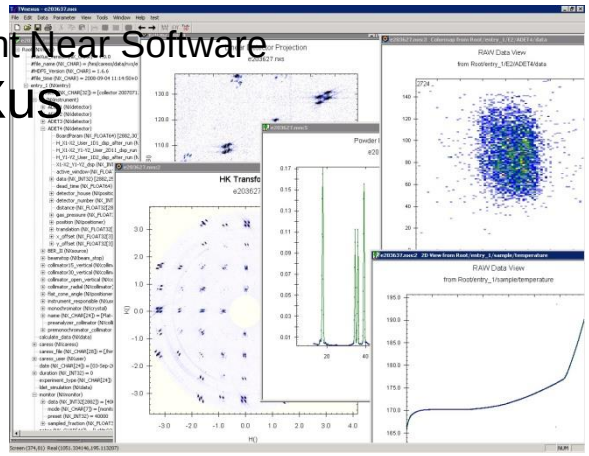
Parameter	Beschreibung
-h, -?, -help	Zeigt eine Hilfe über die verwendbaren Kommandozeilenparameter an.
Programmoptionen	
-iif=<dateiname>	Bezieht die Instrumentkonfigurationsdatei aus <dateiname>.
-isf=<dateiname>	Bezieht die Quellenkonfigurationsdatei aus <dateiname>.
-itp=<Pfadname>	Gibt einen Pfad zum einem (temporären) Verzeichnis an (Standard ./) -> ab Version 2
-of=<dateiname>	Schreibe die NeXus–Daten in die Datei <dateiname>.
-xml Schreibe	die NeXus–Daten als XML–Datei und nicht als HDF5–Datei.
-un=<dateiname>	Schreibt undefinierte Einträge in <dateiname>
Threadoptionen	
-t=<Zahl>	Setzt die maximale Anzahl an gleichzeitigen Threads (Standard sind 10).
-dt=<Zahl>	Setzt die maximale Anzahl an gleichzeitigen Datenakquisitionsthreads (Standard sind 5).
-tt=<Zahl>	Setzt die maximale Anzahl an gleichzeitigen Datenkonvertierungsthreads (Standard sind 5).
-at=<Zahl>	Setzt die maximale Anzahl an gleichzeitigen Datenanalysethreads (Standard sind 5).
Debugoptionen	
-a, -aon	Fügt Debugdaten an das Ende der Log–Datei an.
-aoff	Verhindert das Anhängen von Debug–Daten an die Log–Datei.
-l=<Dateiname>	Schreibt eine Log–Datei (mit dem Standard–Debug–Level 5).
-loff	Verhindert das Schreiben einer Log–Datei.
-son, -soff	Aktiviert / Deaktiviert die Debug–Ausgabe auf dem Bildschirm.
-v=<1-5>	Setzt das Debug-Level auf 1-5 (Standard ist 5) und gibt damit die Wichtigkeit der Debug–Nachrichten an.
Freie Parameter: Beispiele für Standard Source Datei	
0	Caress-Dat File

Instrument PC: ./datacollector /hmi/caress/data/e201234.dat

Data Analysis

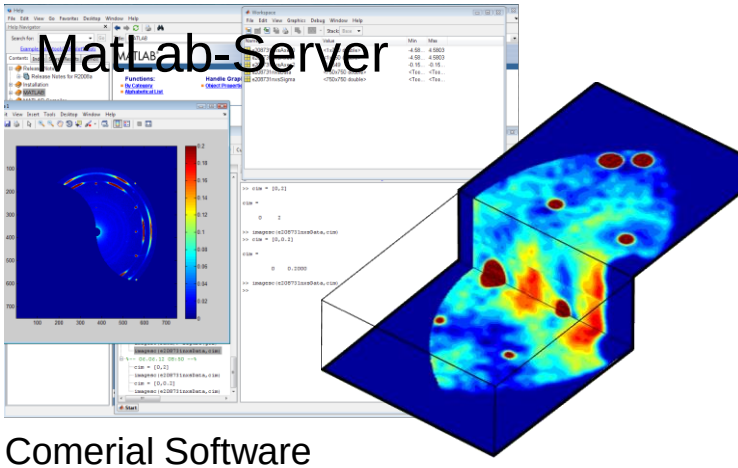
Instrument Near Software

TVneXus



WinServer-Link

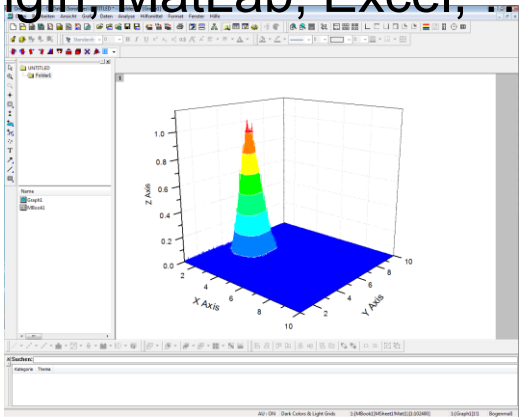
MatLab-Server



Clipboard

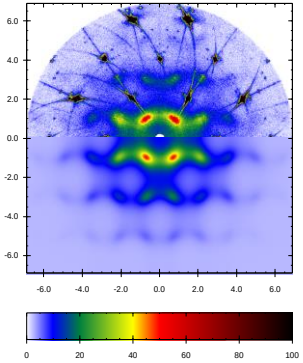
Comerial Software

Origin, MatLab, Excel, …



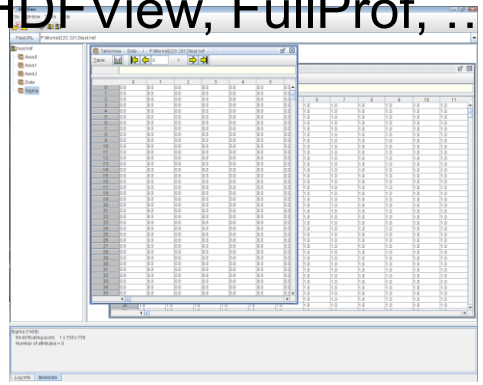
Export HDF, ASCII, …

Internal Fit Functions

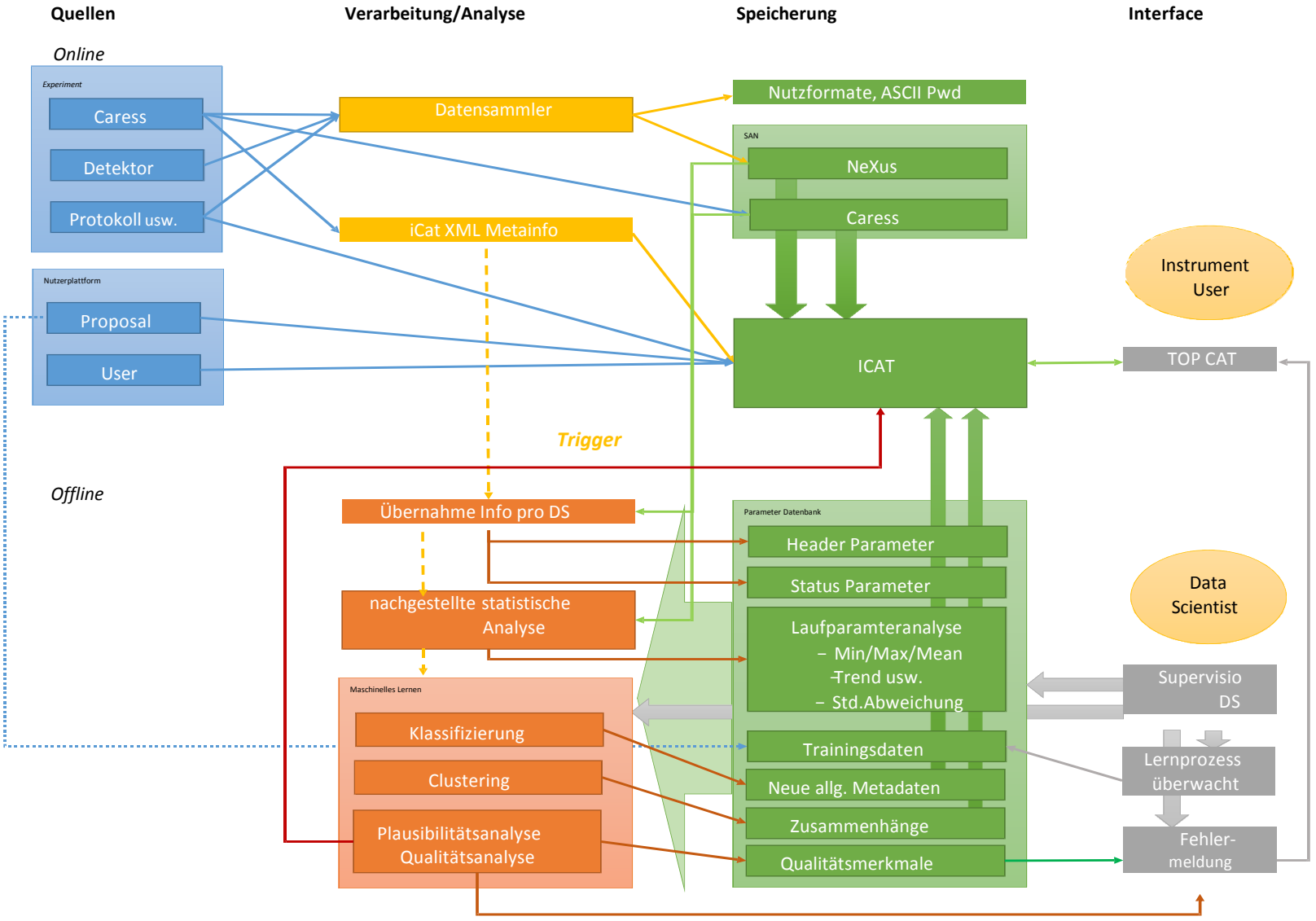


Other Software

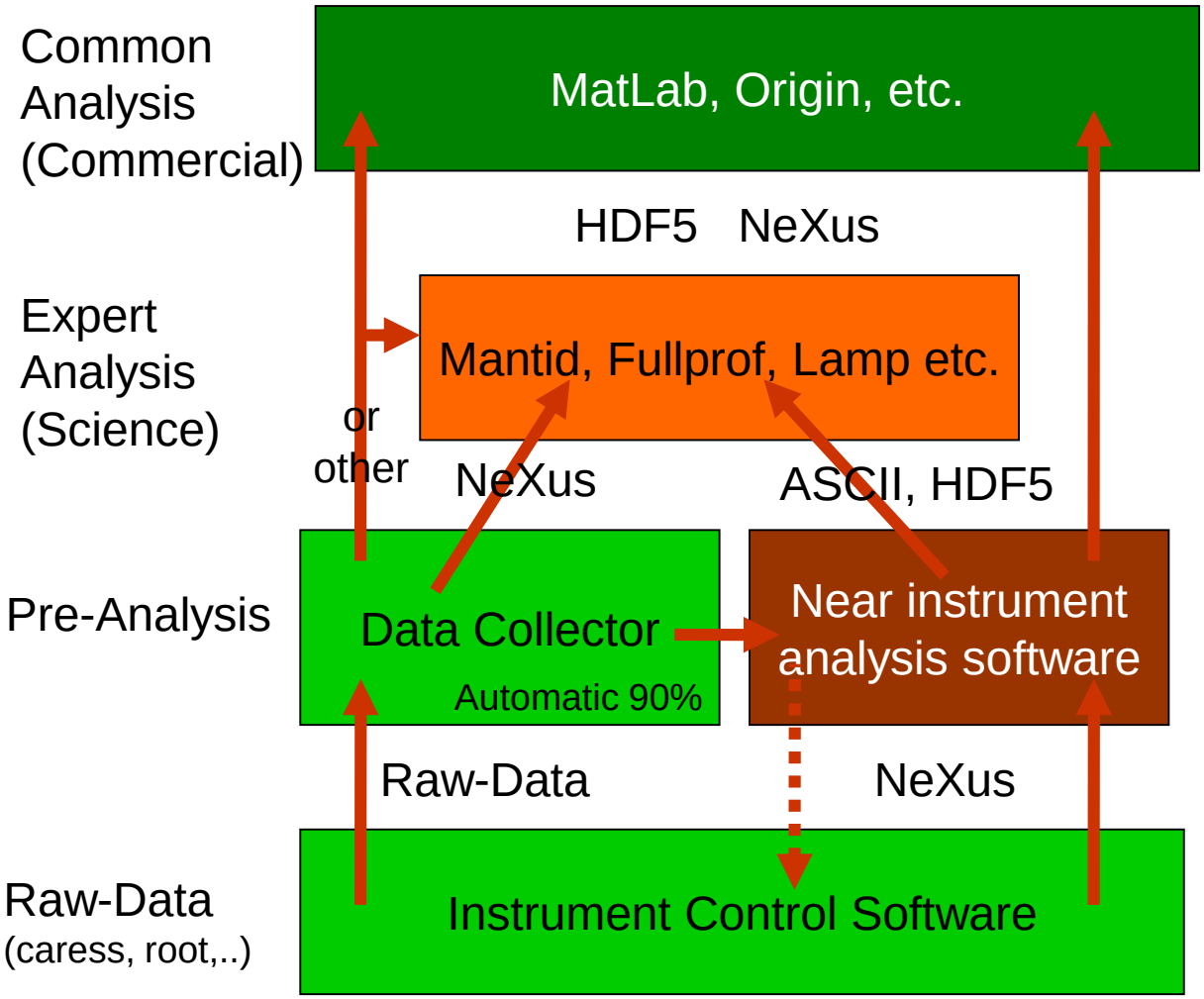
HDFView, FullProf, …



Novel Maschine Learning Approach



Data Handling Concept



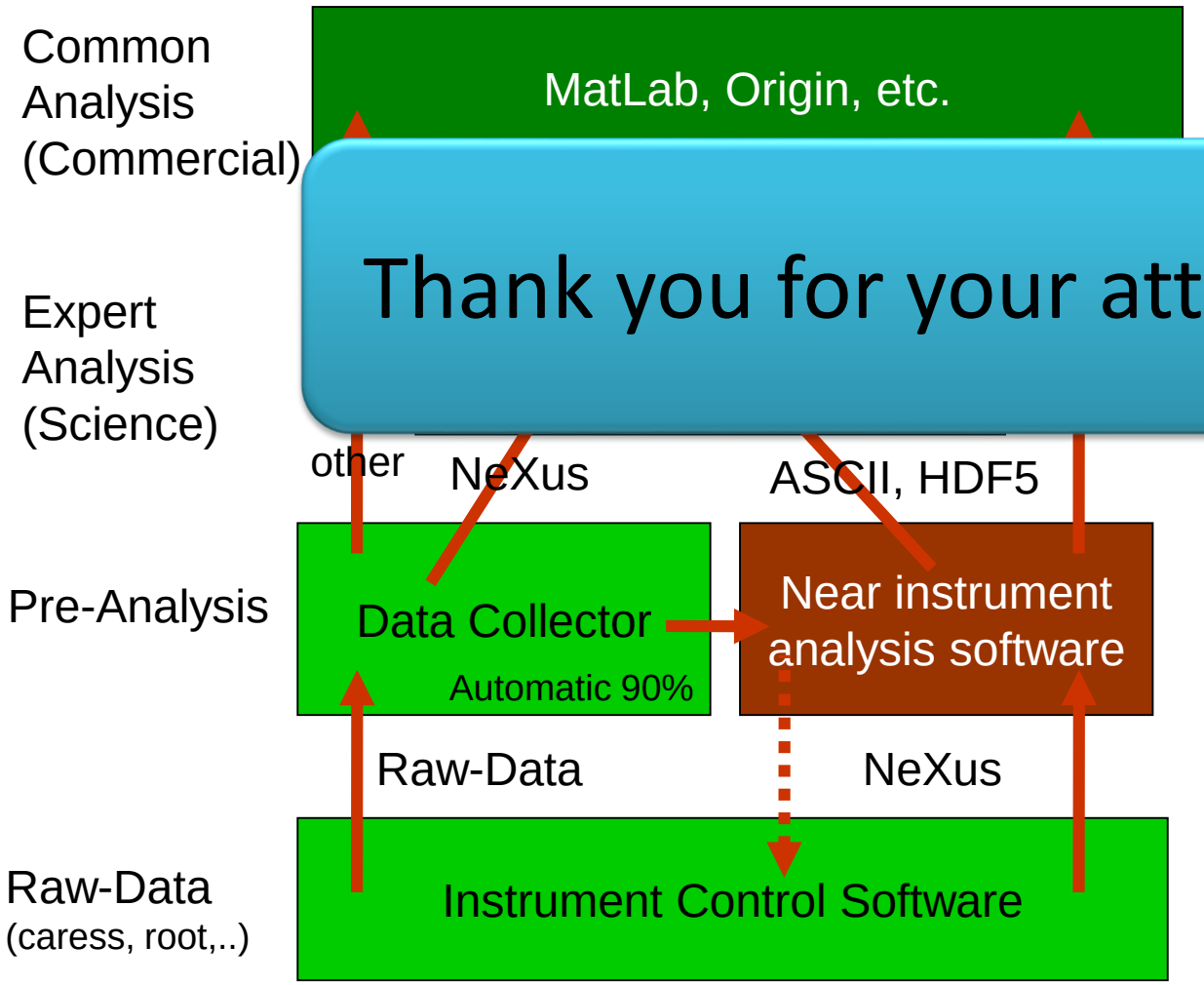
NXprocess/NXdata

entry:NXentry
  sample:NXsample
  processing_name:NXprocess
  program
  version
  parameters:
    NXparameter
  raw_file
data:NXdata
  data[nx,ny,nz]

NXinstrument

entry:NXentry
  sample:NXsample
  instrument:NXinstrument
    source:NXsource
    velocity_selector:
      NXvelocity_selector
    detector:NXdetector
    data[xsize,ysize], signal=1
  control:NXmonitor

Data Handling Concept



NXprocess/NXdata

entry:NXentry
  sample:NXsample
  processing_name:NXprocess

NXinstrument

entry:NXentry
  sample:NXsample
  instrument:NXinstrument
    source:NXsource
    velocity_selector:
      NXvelocity_selector
    detector:NXdetector
    data[xsize,ysize], signal=1
  control:NXmonitor