Virtual Instrument Representation in X3D and some CIF->XML stuff.

Doug du Boulay,

Materials and Molecular Structure Network,

University of Sydney

Virtual Diff. evolution

J. Appl. Cryst. (1995). 28, 225-227.

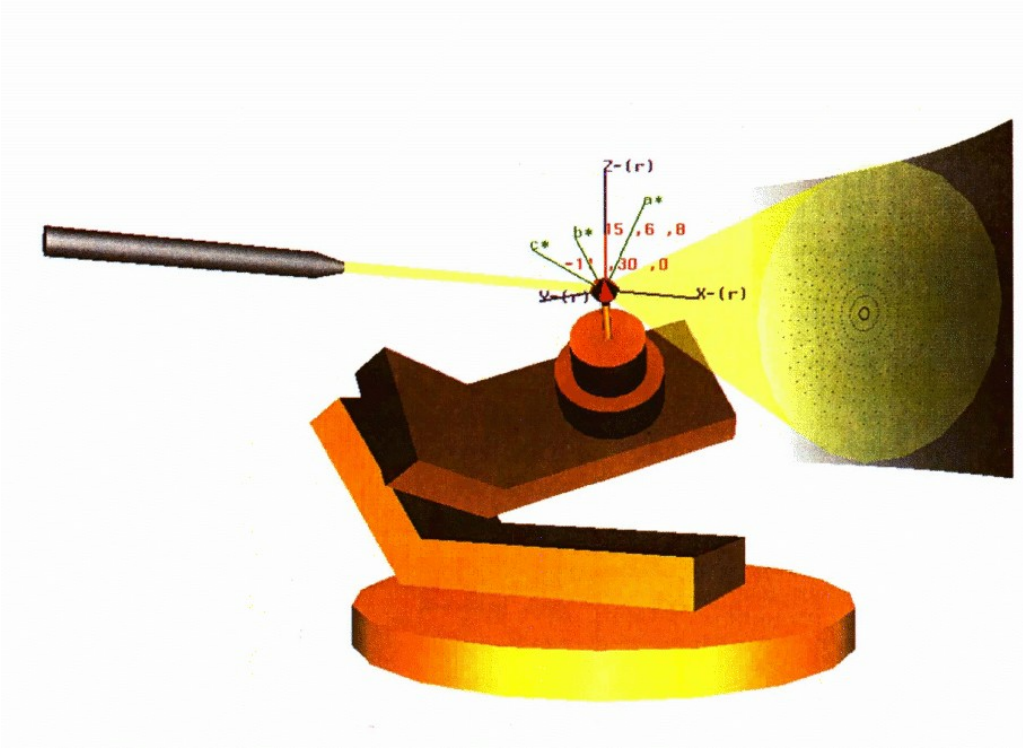
Min Yao, Hokkaido University

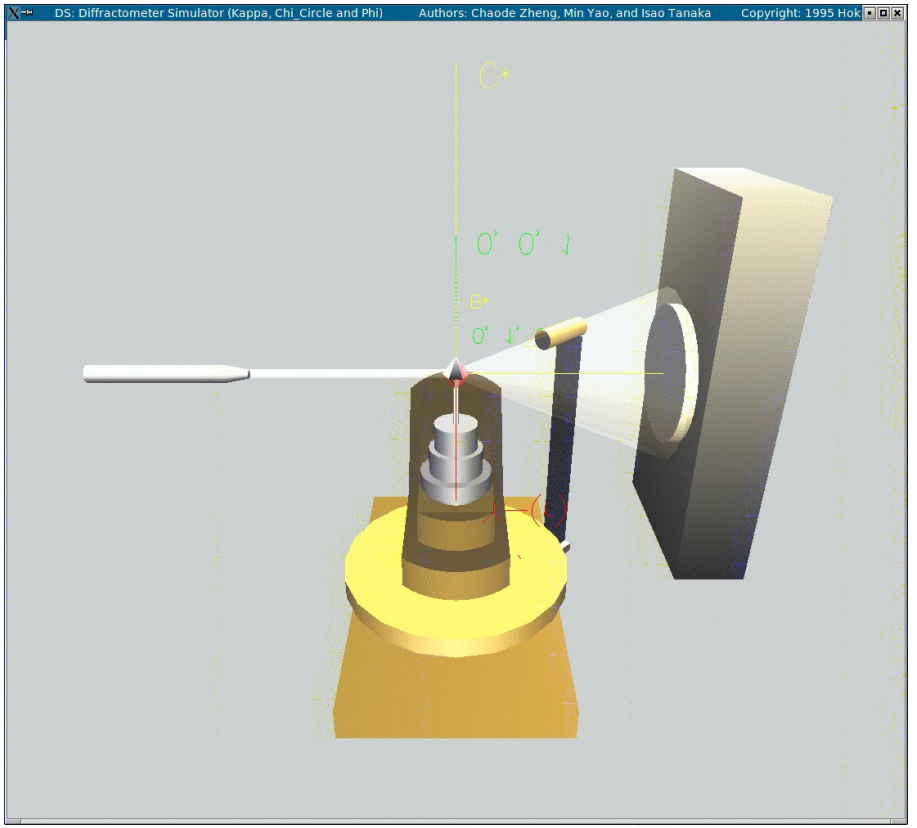
C code program
SGI Iris GL (Graphics Library – predates OpenGL 3D graphics library)
Displays kappa and 4 circle X-ray diffractometers.
Also displays observed reflection listings from a file ...?

ESRF (Min Yao + Darren Spruce)

adapted for use on HP computers,
updated to OpenGL for 3D graphics,
uses tcl/tk for the GUI,
also uses tcl pipes for communication with beamline.
Used to display/monitor beamline status. control ? dunno.
Support for about 6 different diffractometer geometries.

original & ESRF versions





new - Java

Translated Min's C-code to Java.

JOGL JNI to OpenGL libraries

Minimalist Java Swing GUI

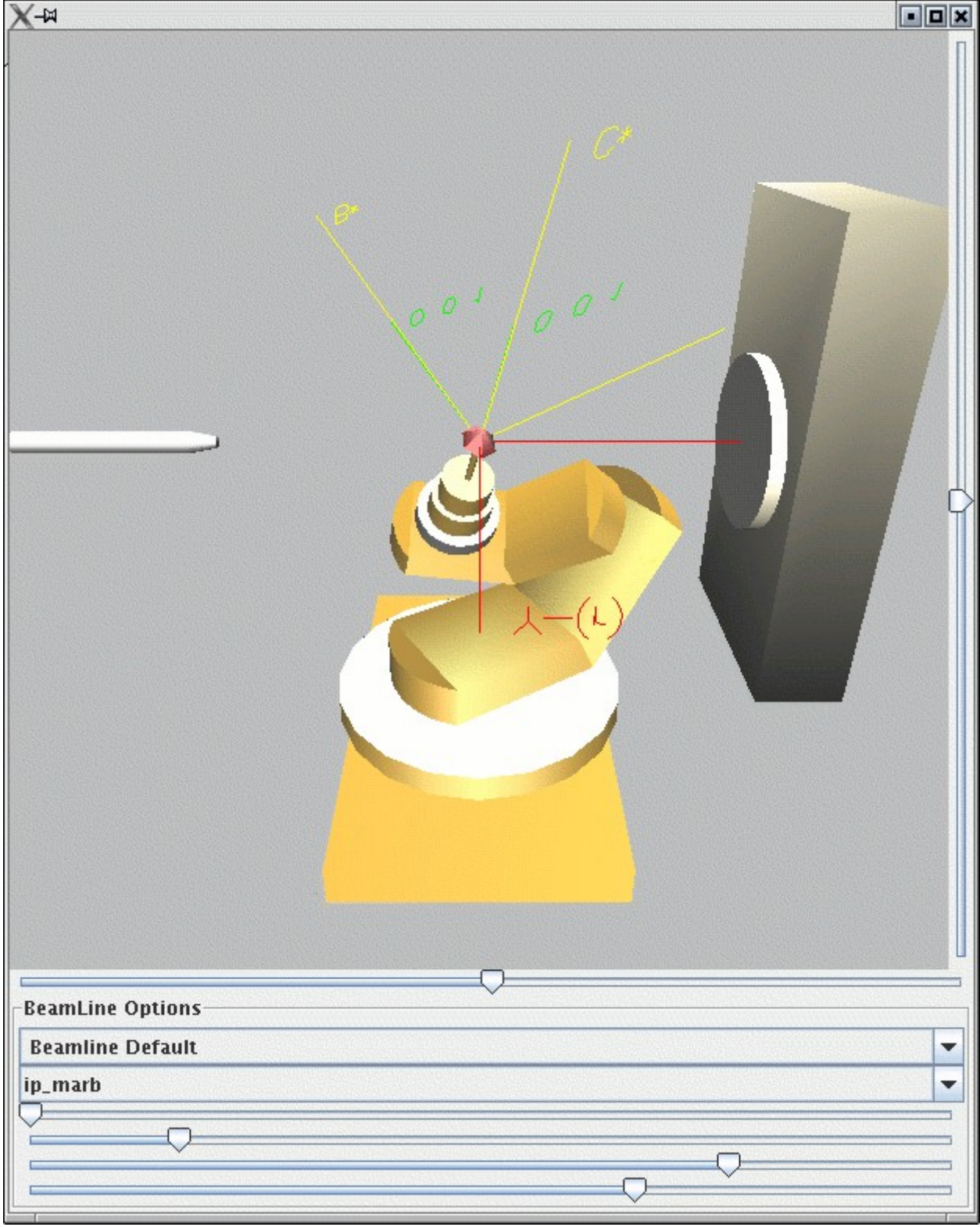
useable as an Applet, or
Java application.

Diffractometer Status Monitoring

HTTP server communication using:

PUSHLETS

Pseudo-realtime display updates.



OpenGL - the sad truth

Very low level code:

```
public static void draw_diskz(GL gl, float r, float[] center, float shifx, float shify, floa
t[] vect, int divid, int start, int  end) {
        int   i;
        float x,y;
        float n[] = new float[3];
        float v[] = new float[3];

        gl.glBegin(GL.GL_TRIANGLE_FAN);
        gl.glNormal3fv(vect, 0);
        v[0] = center[0] ;  v[1] = center[1];  v[2] = center[2];
        if (divid == 40) {
            for (i = start;  i <= end;  i++)  {
                if(i == divid ) { x = cons40[0][0]; y = cons40[1][0]; }
                else           { x = cons40[0][i]; y = cons40[1][i]; }
                v[0] = x*r-shifx;  v[1] = y*r-shify;
                gl.glVertex3fv(v, 0);
            }
        }
      gl.glEnd();
}
```

Construct all diff. components algorithmically -
Decompose cylinders, etc into triangles with vertex normals for correct shading.

- Repeat: adjust, recompile, execute ....

Time consuming/tedious/mundane

Higher level approaches

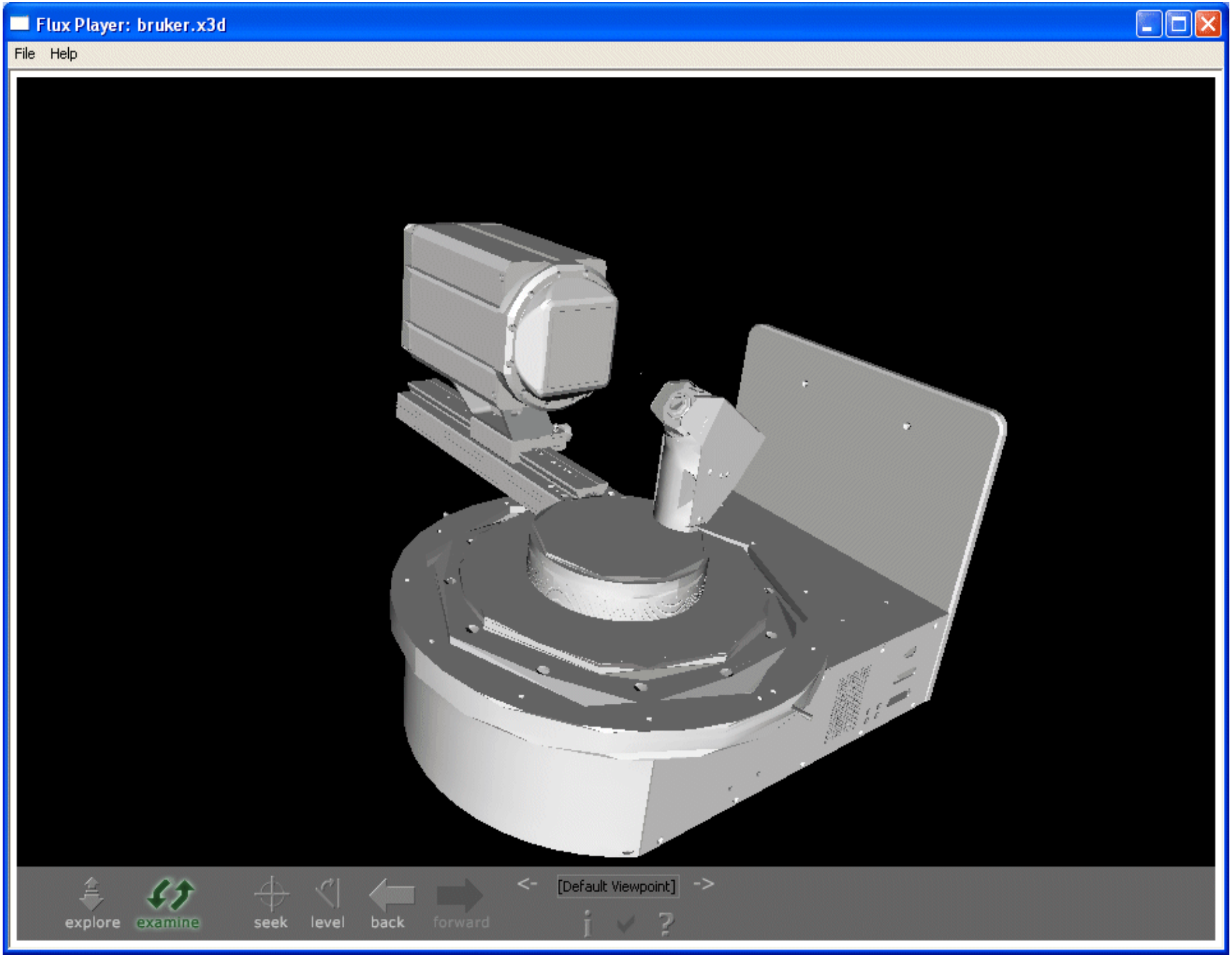
3DS 3D studio
DXF used by AutoCAD
FLT openflight
IGES Initial Graphics Exchange Specification
IV Open Inventor
LWSC Lightwave Scene
MGF Materials and geometry format
OBJ wavefront advanced visualizer object file.

U3D universal 3D format Intel + ...

3DXML - Dassault + Microsoft standard
Beyond Tomorrow: Dassault Falcon Jet aeroplane:
designed/modelled/simulated entirely in VR

Solid Works (perhaps the best commercial option???)
a standard for autoCAD/CAM
as well as physics simulation

STEP format supplied by Bruker - vastly more detail than we need for simulation.


Flux Player: bruker.x3d
File
Help
explore
examine
seek
level
back
forward
<-
[Default Viewpoint]
->
i
?

Virtual worlds?

Proprietry 3D virtual world formats

activeWorlds.com
Blaxxun Interactive
Worlds.com
SecondLife.com

Alternatively: VRML or X3D

advantages:

ISO standard!
scripted text file,
relatively easy to read and edit.
several free players/browsers
free editor
X3D has an XML format – can play nicely with other XML dialects.
(namespace issues ???)
Open flexible, evolving spec -
different possible levels of support

VRML/X3D

Web3D consortium - the driving force behind VRML

VRML1 ~1994
SGI Open Inventor

VRML2 = VRML97 also an ISO standard
SGI Cosmo Player
cortona

X3D
Also includes a spatial audio spec.

Octaga Windows only + browser plugin
Flux Player Windows only + browser plugin + SAI
Xj3D modular Java based - uses JOGL or Java3D or Mobile 3D
- no plugin, no external SAI primary development horse of Web3D.
FreeWRL Canada Gov. for linux + OS X - soon expected external SAI
written in C and Java, uses OpenGL
firefox plugin support

Creating X3D models

manually - written by hand

manually – with application specific editor e.g. X3D-Edit

Graphically -

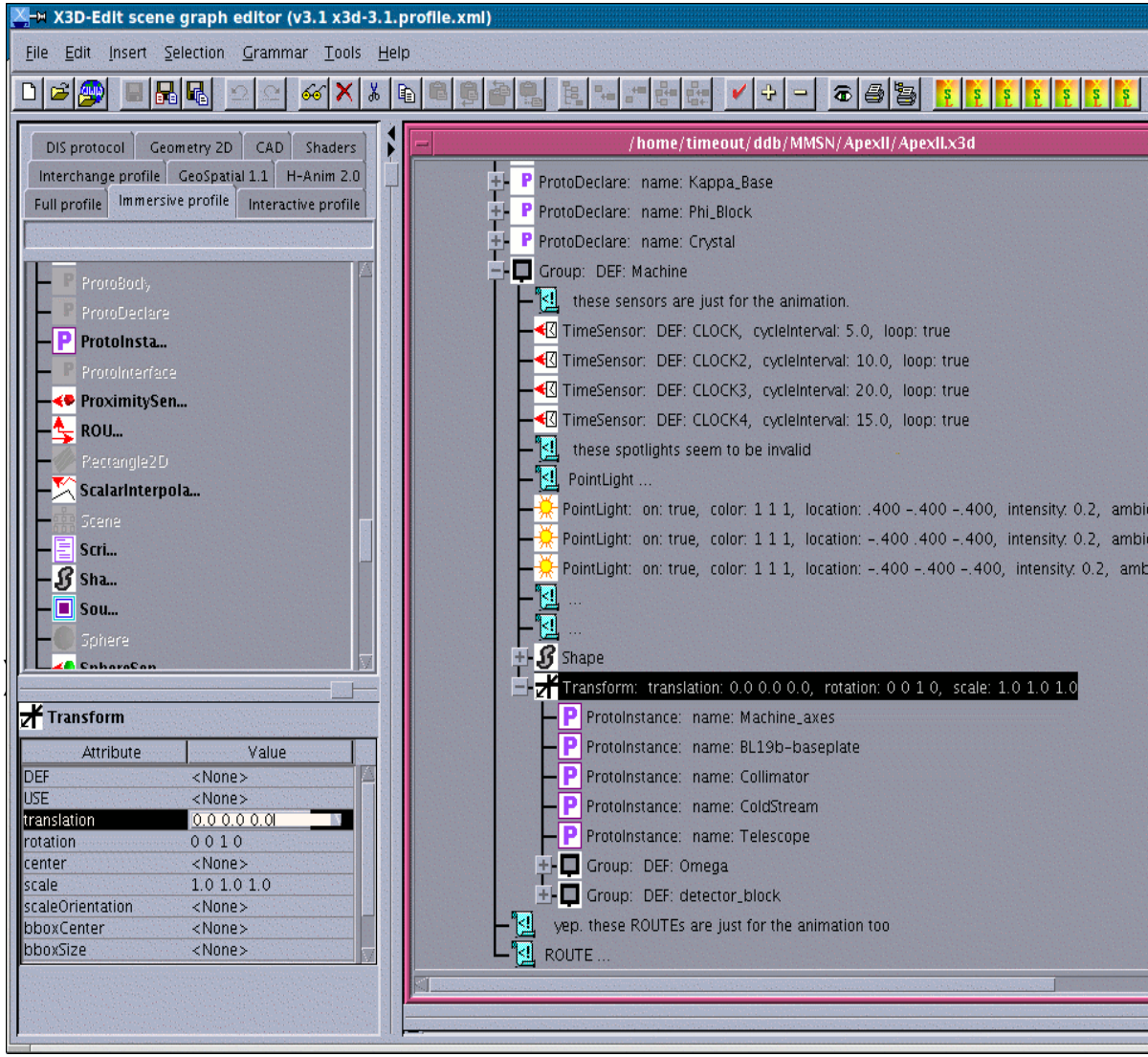
Flux Studio beta download – free – but some features from the core spec are missing.

Amaya has an X3D exporter.

Blender - free 3D OpenGL modelling tool, (Windows + linux) exports VRML1 - transformable to VRML2 and then X3D.

Downside?

Can't really think of any.



X3D profiles

core
absolute minimalist graphic primitives implementation

interchange
exchange of geometry between authoring systemms
no user interaction
simple viewers
simple lighting models

interactive profile
limited navigation and environment sensors
immersive profile
for immersive virtual worlds
including navigation and environment sensors
full profile
all features of the X3D standard

Extended Profiles

geospatial
optimzation for mapping and 3D terrain models

Human animation
abstract representation for modelling 3D human figures
including joint limitations

programmable Shaders
to increase realism

CAD
intended for interchange of CAD data
materials
textures
simplifies complex objects down to simple ones.

Distributed Interactive Simulations
aka. networked modelling & simulation

several others.

Extension elements? attributes ? -unrecognised/unsupported

X3D XML structure

```
<X3D profile=”?”>
  <head>
   <meta />
  </head>
  <scene>
    <background />
    <navigationInfo />
    <viewpoint />
    <protodeclare   name="some fundamental/reusable scene component">
                  also externalProtos loaded from URL bank/library       - instrument ontologies?
      <protobody>
        <group>
          <transform>   nested arbitrarily deep
            <group>
              <transform>
                <shape>
                  <appearance>
                   graphics primitive     e.g. box, sphere, cylinder,  indexed face set,   triangle strips etc
    </protodeclare>
    <protodeclare>...</protodeclare>

    <group>
      <sensors>    time sensors= alarms,   pointing device sensors,  drag,  touch sensors,  environment sensors
      <lights>
      <shapes>
      <group>
        <transform DEF="UNIQUE_ID" translations, rotations, scales>
          <protoinstance>
          <interpolators  - orientation, position scalar ...>

   </group>

   <routes>  from sensor to interpolator
           from interpolator to node ( transform or color  or ...)
  </scene>
</X3D>
```

Script Nodes!

Supporting Javascript, or Java (class URLs)

- Can manipulate internally via the Scene Authoring Interface (SAI)
- Also externally, through exported SAI, (only in Flux)

```
<Transform translation="-2.3 2 0">
  <Shape>
    <Appearance>
      <Material diffuseColor="0 0 0" emissiveColor="0 0 0"/>
    </Appearance>
    <Text DEF="LOGO_TEXT">
      <FontStyle USE="TEXT_STYLE"/>
    </Text>
  </Shape>
</Transform>

<Script DEF="LOGO_SCRIPT">
  <field name="Logo" type="MFString" accessType="outputOnly"/>
  <![CDATA[ ecmascript:
    function initialize() {Logo[0] = Browser.getName() + ' ' + Browser.getVersion();}
  ]]></Script>
<ROUTE fromNode="LOGO_SCRIPT" fromField="Logo" toNode="LOGO_TEXT" toField="string"/>
```

DS X3D updated by streaming pushlet - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://mmsngate.chem.usyd.edu.au:8051/simulator/

X3D Based Diffractometer Simulator

(driven entirely by javascript and requiring the Flux Player)

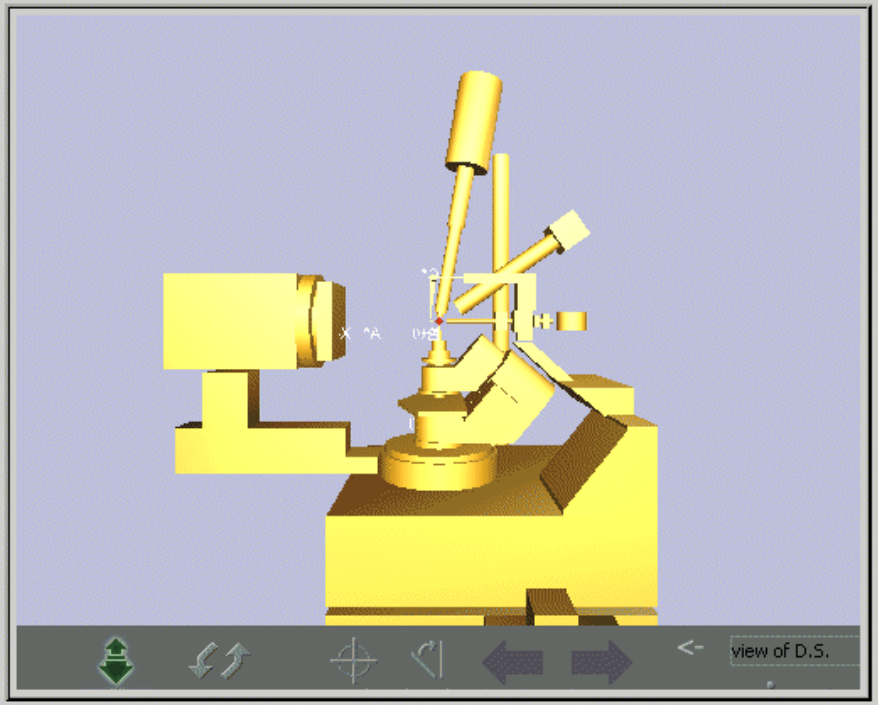
2 Theta (θ):	0.00	(-180 ... +180°)
Omega (ω):	0.00	(-180 ... +180°)
Chi (χ):	0.00	(-100 ... +100°)
Phi (φ):	0.00	(0 ... 360°)
Detector Distance:	170	(32 ... 310mm)

Drive Get Node refs Reset

speedup: 1

Auto delay: 300 (s)

X3D duty-cycle: 3



Status

```
phi undefined kappa
undefined omega
undefined theta
undefined detector
undefined context
[object NPObject JS
wrapper class]
```

Collection Strategy

scan	distance	2 θ °	ω °	φ °	χ °	width °	sweep °	direction
omega	50.20	-28.80	-15.00	0.00	54.74	5	130	-
omega	50.20	-28.00	-15.00	120.00	54.74	5	130	-
omega	50.20	-28.00	-15.00	240.00	54.74	5	130	-
omega	50.20	-28.00	40.00	0.00	-54.74	5	80	-
omega	50.20	-28.00	40.00	120.00	-54.74	5	80	-
omega	50.20	-28.00	40.00	240.00	-54.74	5	80	-
phi	50.20	24.00	25.47	-11.45	-26.64	5	360	-

all Examine Pause Resume Abort

Done

Pushlets

Java servlets with persistent state, running within a web server.

Allow server to client communication over HTTP by opening up a file stream connection that never terminates.

Server state is periodically, or intermittently broadcast to listening clients by dumping info into the connection pipe,
iether as an XML packet,
or as javascript code -to be parsed or evaluated by the client.
Keepalive packets also.

Consequently, we can communicate diffractometer settings and status from the web server to the client through most firewalls and over ordinary HTTP connections.

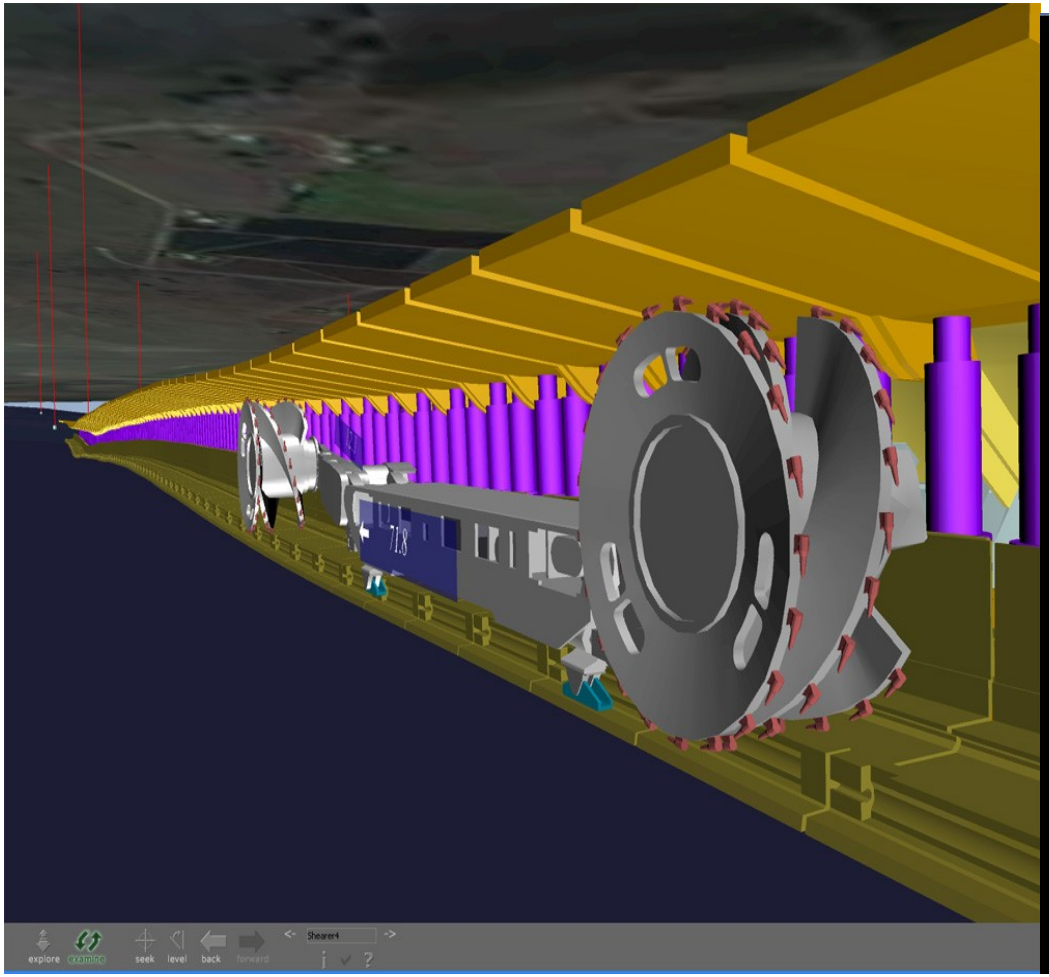
ALSO: HTTP clients can publish their own status to the server, which then rebroadcasts
to all listening clients.

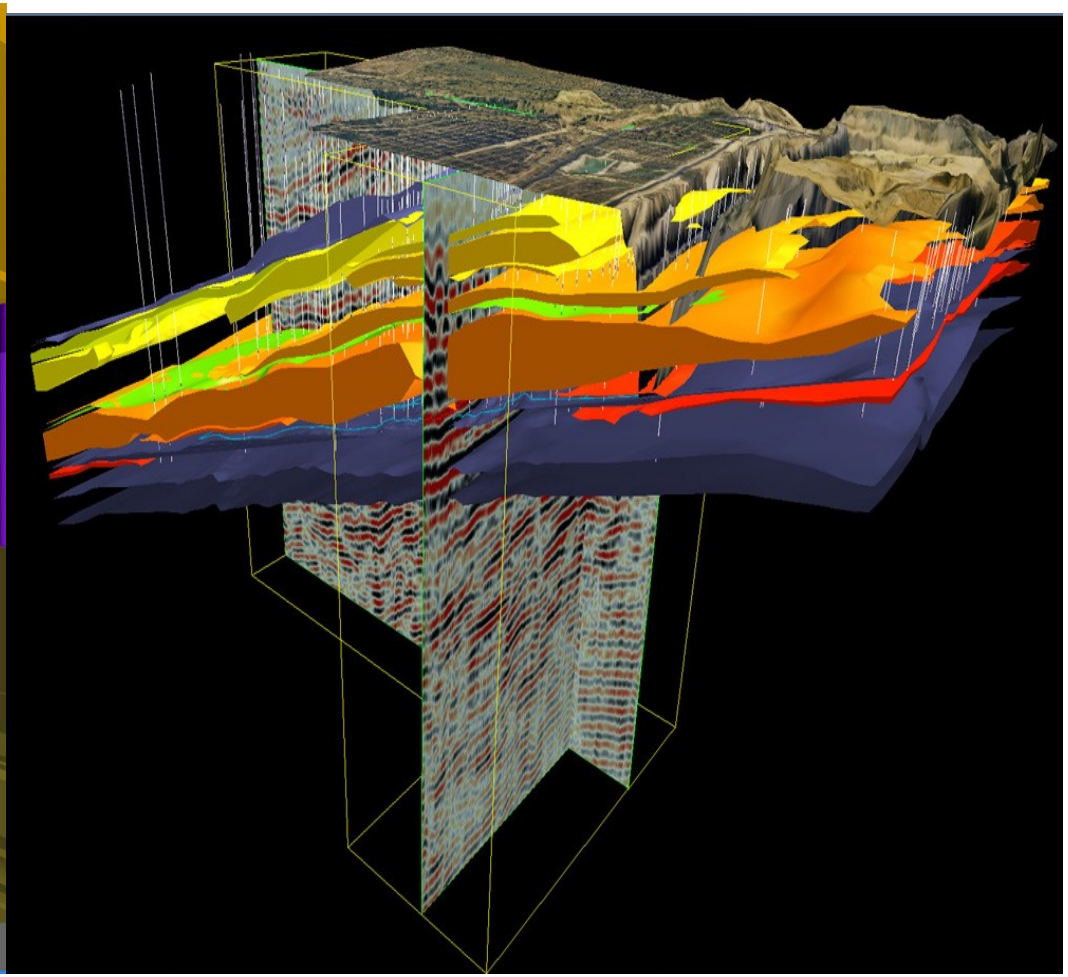
POT HOLES: -

- if we only receive settings at start and finish of diffractometer motion
  - BIS problems
- Sometimes the streaming connection will be broken – but reestablished,
  - losing state info?
- IE only supports 2 simultaneous server connections (!???)

Con.Caris@csiro.au

Stream real-time sensor data, over a thousand kilometers through secure VPNs (24 x 7), from large scale underground mining equipment, directly into 3D worlds. Model is monitored remotely using a Java application built around Flux Player.





X3D outlook?

Xj3D Java X3D browser

Can be embedded in a Java Applet/ Application and driven by pushlets.

Can use cell orientation matrix to calculate / display observable reflections - compare with CCD/imageplate images.

Picking extension for collision detection (not so good as yet)

Instrument collision map?

CIF to XML???

2000 work with Syd Hall/Spadaccini/Castleden on DDL3
New programming language dREL
(CIF dictionary Relational Expression Language)
Add evaluation methods to CIF data name definitions
for validation, or to evaluate missing data items.
(Permitted but never implemented in DDL2 - potentially written in many different programming languages, whereas DDL3 would have just one - potentially mapped/transformed into different languages/libraries on demand)

CIF 1.0 data representation - is quite limiting
limited to single values or tables of values
(STAR is more powerful, but little software exists)
for extensive data tables requires new names for things that don't deserve them i.e. columns in large matrices

CIF 1.0 documentation - Promoted as a journal article submission format.
Crude typesetting info embedded in the text.
No semantic information.

CIF 1.0 seems to be 1/2 a data container with 1/2 a documentation container => 1/4 the power of XML (as an upper limit)?

CIF 2.0 == DDL3 - support for matrices and lists ? dunno...

CIF dictionaries ->DocBook

Experience with DocBook, while working on Xtal System.

Mapped the DDL0, DDL1, DDL2 and experimental DDL3 dictionaries into a DocBook XML variant - using James Hester's PyCifRW CIF reader and python.

Dictionaries become explicitly hierarchical – (good or bad - grouping?)
Can contain figures and equations and maintain extensive cross references and bibliographic and citation information and indices and tables of contents.

DDLs to describe the CIF dictionaries are also self descriptive,
- can function as there own reference documentation.

XML is ugly, BUT we can map the DocBook dictionary into HTML or PDF using some quite well supported free publishing tools.
(tedious to write directly in XML)

Equally, for current use, these documents can be XSLT transformed back to standard CIF dictionary format.

Alternative DDL3 XML languages for describing algorithms include MathML, OpenMath, UnitsML? Numerical Math Consortium

CIF files ->DocBook + XDF

Single-sourcing - one source of data and documentation – evolving in synch?
OpenOffice.sxw format is a zipped file of styles and documents and figures, so ?

Map CIF journal submission data into DocBook XML with an XDF supplement.
DocBook - reasonably generic documentation format
(see also modular Darwin Information Typing Architecture DITA topicmaps)
(not 100% *kosher* DocBook, but very close)
XDF – generic XML data format developed by NASA for Astro. data.

Map CIF text into LaTeX, then apply a crude text parser
to identify semantic information - chemical formulae, citations,
figure and table references for cross linking, componentised bibliography data.

Journal publishing -> one-off transform to web/PDF,
but XSLT can remap source doc -as required -across whole website to
improve renderring, change style or add new behaviours for more dynamic web pages.

UK All Hands eScience meeting August 06:
P.M.R. Cambridge extensive (== several research groups) effort to mine existing published PDF literature for chemical info, using character recognition and “Natural Language Processing”.

Alternatively – we could inject semantic info (RDF/A) from the beginning for new documents.

Latent interest in contributing to imgCIF and NeXuS -

New connections with ESRF and FABLE project?

http://fable.sourceforge.net/

ImageCIF and Java based CCD image analysis?