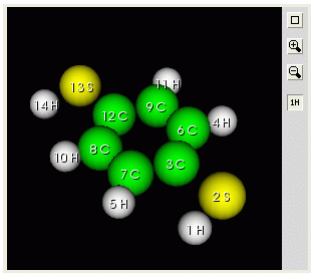
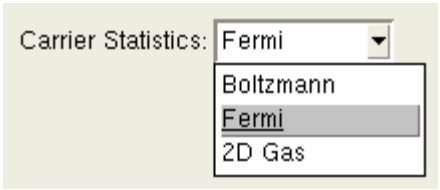
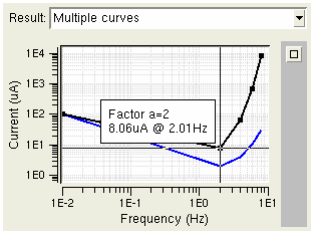
nanoHUB online simulation and more — an NCN project

Advanced Rappture Concepts







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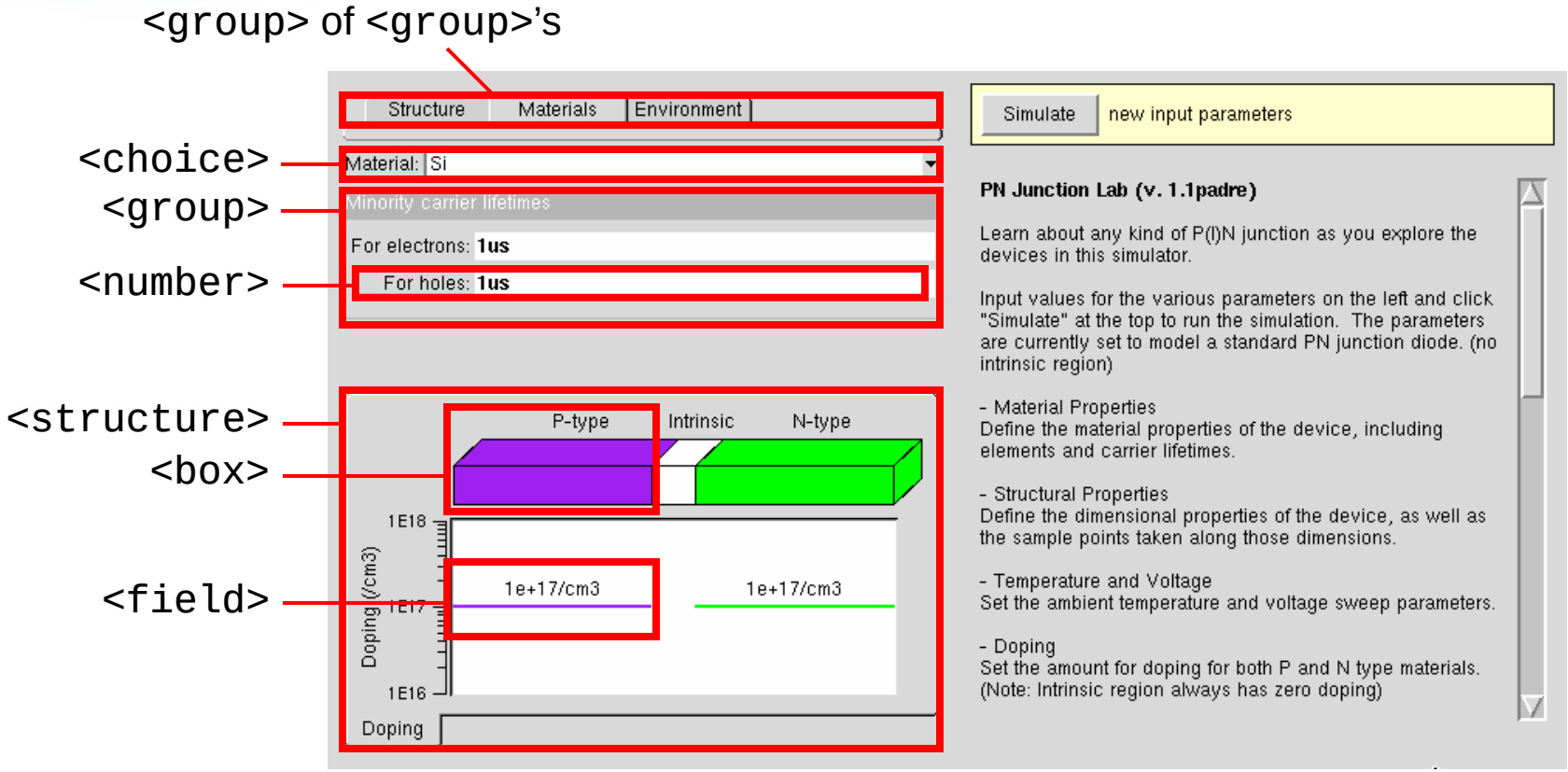
NCN NSF

Identify the elements



<structure>

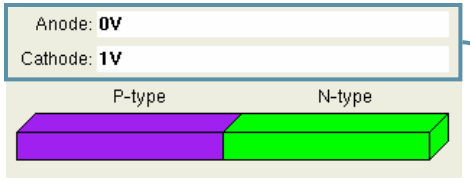
Structure of physical system being simulated

Just 1-D boxes, for now

```
<structure>
  <current>
    <components>
      <box>
        <about>
          <label>P-type</label><color>purple</color>
        </about>
        <corner>0</corner>
        <corner>0.1um</corner>
      </box>
      <box>
        <about>
          <label>N-type</label><color>green</color>
        </about>
        <corner>0.1um</corner>
        <corner>0.2um</corner>
      </box>
    </components>
  </current>
</structure>
```

<structure>

Structure of physical system being simulated

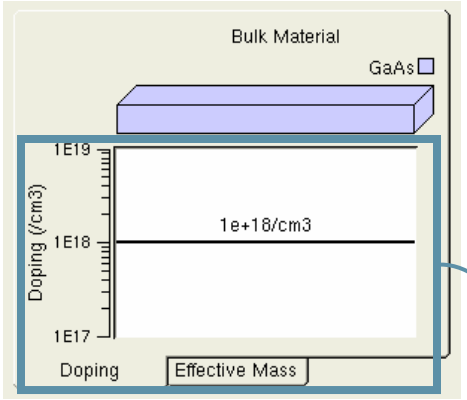



```
<structure>
  <current>
    <parameters>
      <number>
        <about><label>Anode:</label></about>
        <units>V</units>
        <default>0V</default>
      </number>
      <number>
        <about><label>Cathode:</label></about>
        <units>V</units>
        <default>1V</default>
      </number>
    </parameters>

    <components>…</components>
  </current>
</structure>
```

Same as before

<structure>

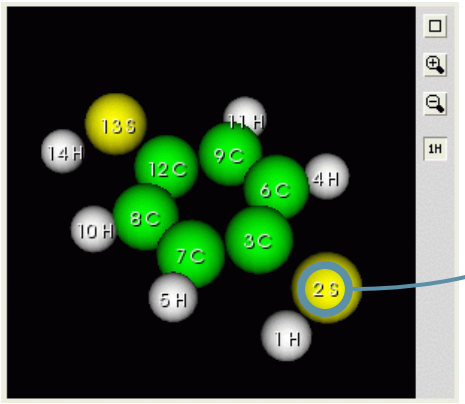
Structure of physical system being simulated




```
<structure>
  <current>
    <units>um</units>
    <parameters>
      <number id="doping">…</number>
    </parameters>
    <components>…</components>
    <fields>
      <field>
        <about>
          <label>Doping</label>
          <color>black</color>
          <scale>log</scale>
        </about>
        <units>/cm3</units>
        <component>
          <constant>doping</constant>
          <domain>box0</domain>
        </component>
      </field>
      …
```

<structure>

Structure of physical system being simulated

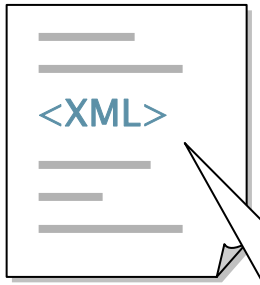


Turns atom labels on by default

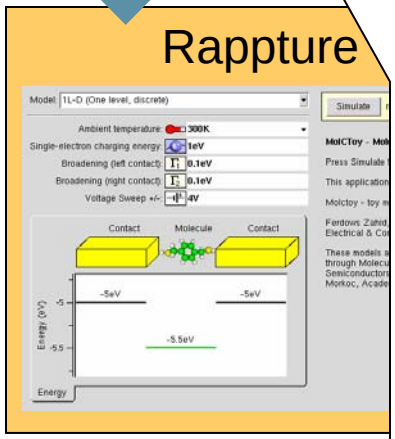
```
<structure>
  <current>
    <components>
      <molecule>
        <about><emblems>on</emblems></about>
        <formula>pdt</formula>
        <atom id="0“>
          <symbol>H</symbol>
          <xyz>-1.24935 -3.41562 0.0</xyz>
        </atom>
        <atom id="1">
          <symbol>S</symbol>
          <xyz>0.08092 -3.19426 0.0</xyz>
        </atom>
        …
      </molecule>
    </components>
  </current>
</structure>
```

Focus on <output> side of tool.xml

description of tool, including inputs and outputs



tool.xml

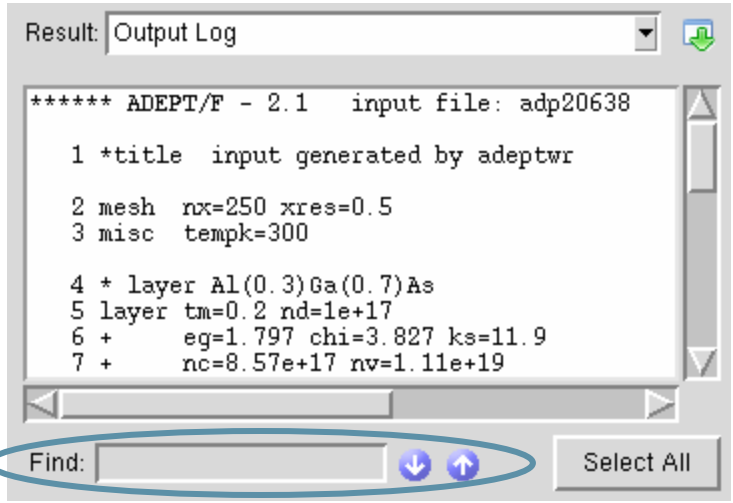



```
<?xml version="1.0"?>
<run>
  <tool>
    <about>This is my tool.</about>
    …
  </tool>
  <input>
    [redacted]
  </input>
  <output>
    [redacted]
  </output>
</run>
```

Produces the user interface *automatically!*

<log>

Standard output from simulator



Controls for search through text

Treated as unimportant (low level) output, and therefore listed last

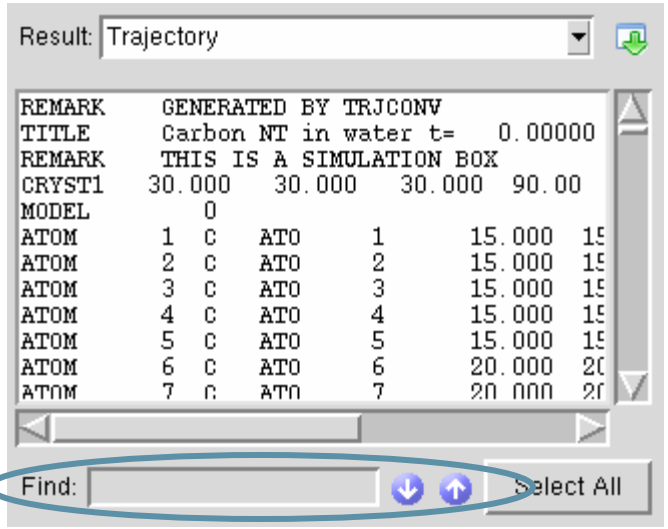
```
<output>
  <log>****** ADEPT/F - 2.1   input
file: adp20638      Sat Jul 30 19:39:36
2005 ******

   1 *title  input generated by adeptwr

   2 mesh  nx=250 xres=0.5
   3 misc  tempk=300
   …
  </log>
</output>
```

or, in Python…

```
import Rappture
import sys
driver = Rappture.library(sys.argv[1])
…
driver.put('output.log', stdout)
```

<string>

Other output files from simulator—including binary files



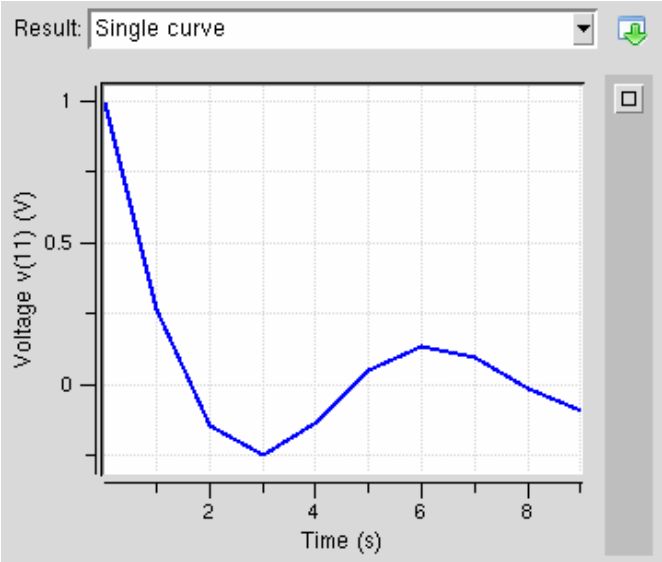
Controls for search through text

```
import Rappture
import sys
driver = Rappture.library(sys.argv[1])
…
path = 'output.string(traj)'
dr
dr
dr
```

```
<output>
  <string id="traj">
    <about>
      <label>Trajectory Data</label>
      <description>Data in pdb
format</description>
    </about>
    <current>REMARK   GENERATED BY
TRJCONV
TITLE     Carbon NT in water t=   0.00000
…
    </current>
  </string>
</output>
```

<curve>

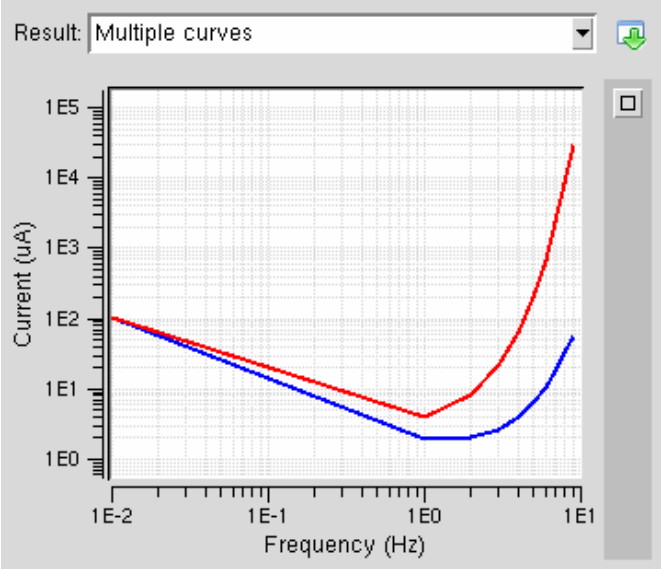
X-Y plots




```
import Rappture
import sys
driver = Rappture.library(sys.argv[1])
…
path = 'output.curve(single)'

driver.put(path+'.about.label',
  'Single curve')

driver.put(path+'.xaxis.label', 'Time')
driver.put(path+'.xaxis.units', 's')
driver.put(path+'.yaxis.label', 'Voltage')
driver.put(path+'.yaxis.units', 'V')

data = """
0 0
1 2
3 4 """
driver.put(path+'.component.xy', data)
```

<curve>

Multiple curves on the same plot



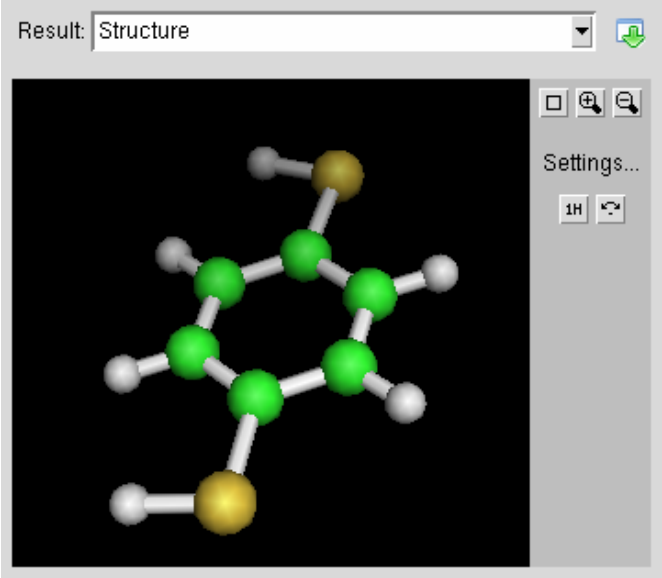

```
import Rappture
import sys
driver = Rappture.library(sys.argv[1])
…
path = 'output.curve(m1)'
driver.put(path+'.about.group',
   'Multiple curves')
driver.put(path+'.about.label',
   'factor a=1')
…
path = 'output.curve(m2)'
driver.put(path+'.about.group',
   'Multiple curves')
driver.put(path+'.about.label',
   'factor a=2')
```

Same group name

Different labels
for different curves

<structure>

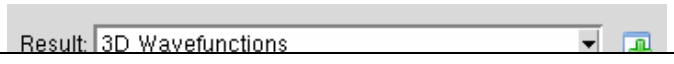
Molecules




```
import Rappture
import sys
driver = Rappture.library(sys.argv[1])
…
path = 'output.structure(mol)'
driver.put(path+'.about.label', 'Structure')

path += 'components.molecule'
driver.put(path+'.atom(0).symbol', 'H')
driver.put(path+'.atom(0).xyz', xyz0)
driver.put(path+'.atom(1).symbol', 'S')
driver.put(path+'.atom(1).xyz', xyz1)
…
```

<field>

Scalar field defined over (x,y) or (x,y,z)




```
import Rappture
```

```
object 1 class gridpositions counts 126 30 22
origin 0.00000000E+00 0.00000000E+00 0.00000000E+00
delta 50.0 0.0 0.0
delta 0.0 50.0 0.0
delta 0.0 0.0 69.0476190476
object 2 class gridconnections counts 126 30 22
object 3 class array type double rank 0 items 83160 data follows
0.28865594E-02
0.28865594E-02
0.28865594E-02
…
-0.71134413E-02
-0.71134413E-02
attribute "dep" string "positions"
object "regular positions regular connections" class field
component "positions" value 1
component "connections" value 2
component "data" value 3
```

nx ny nz

xgrid

ygrid

zgrid

Scalar values:
z-index varies fastest,
then y-index,
then x-index

total number of
data points:
nx * ny * nz

```
y[1])

k', dxdata)
tyle',
city 1')

k', dxdat2)
tyle',
-max 1')
```

<sequence>

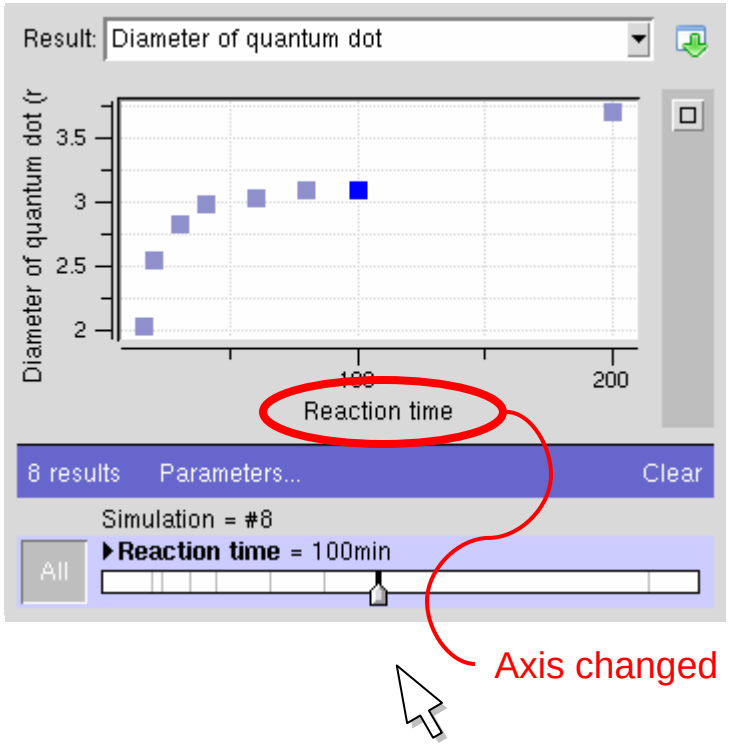
Sequence of images, curves, or fields


```
<sequence id="movie">
  <about>
    <label>Animated sequence</label>
  </about>
  <index><label>Frame</label></index>

  <element id="0">
    <index>1</index>
    <image>
      <current>/9j/4AAQSkZJRgAA…</current>
    </image>
  </element>

  <element id="1">
    <index>2</index>
    <image>
      <current>/9j/4ARgASkZJQQR…</current>
    </image>
  </element>

  …
</sequence>
```

Just like a normal output image

<number> and <integer>

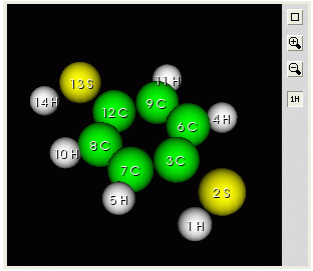
Just a number or integer, but compare across many runs

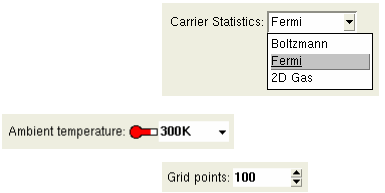



```
import Rappture
import sys
driver = Rappture.library(sys.argv[1])
…
path = 'output.number(d)'

driver.put(path+'.about.label',
  'Diameter of quantum dot')

driver.put(path+'.units', 'nm')
driver.put(path+'.current', d)
…
```

nanoHUB online simulation and more — an NCN project

Tour the zoo





Zoo of Examples

- Complete catalog of data objects online
- See screen shots
- Copy xml code

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