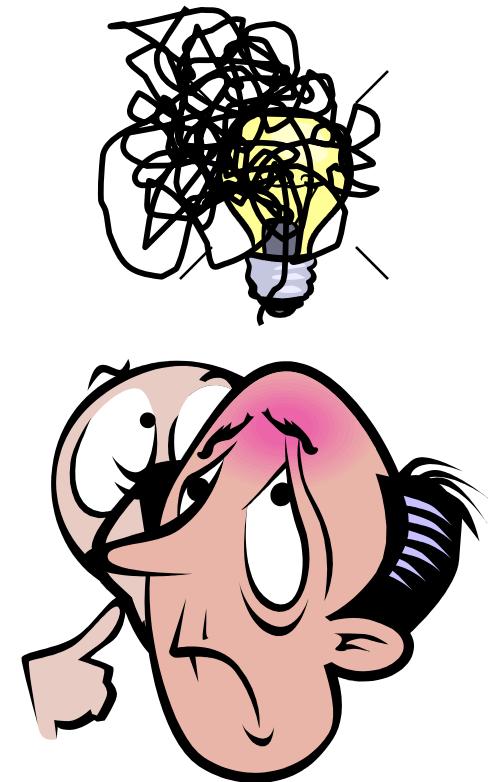
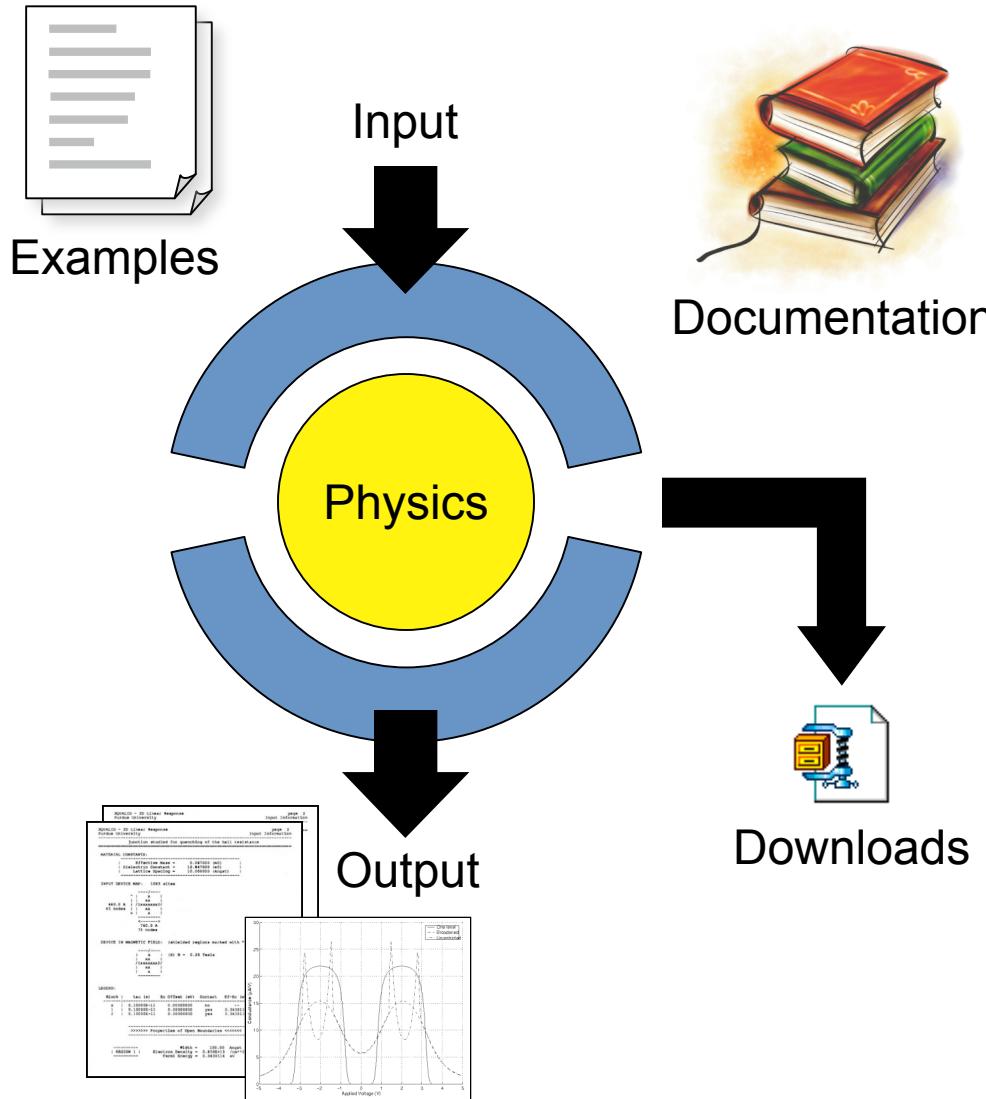
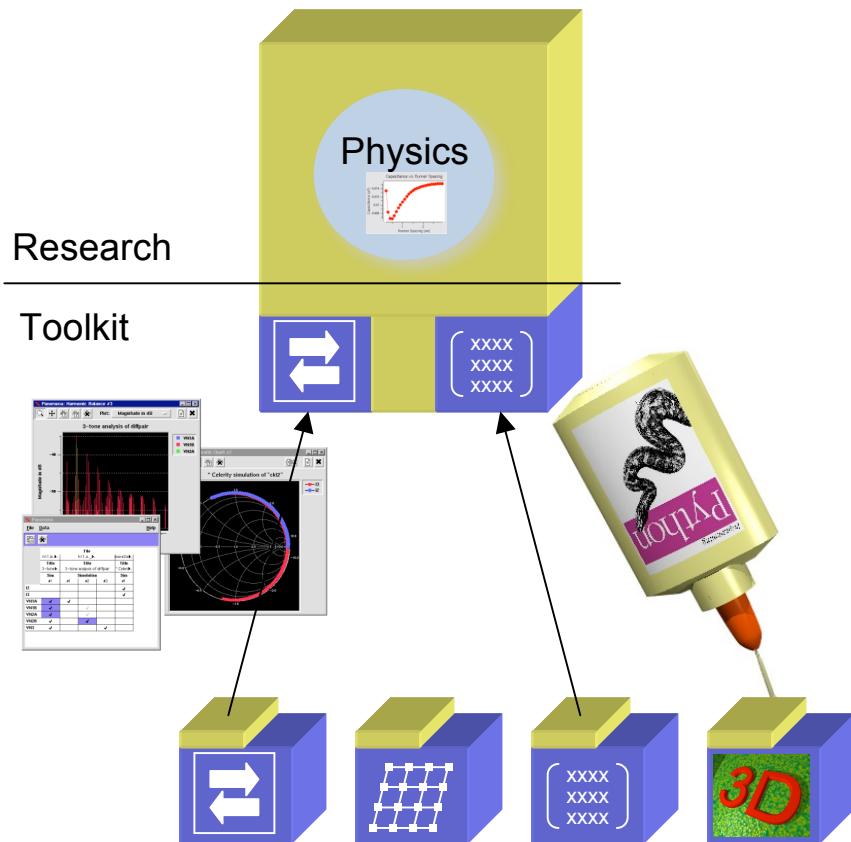


Scientific Computing, Scripting, and Rappture

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Purdue University
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Rappture toolkit → Rapid Application Infrastructure toolkit



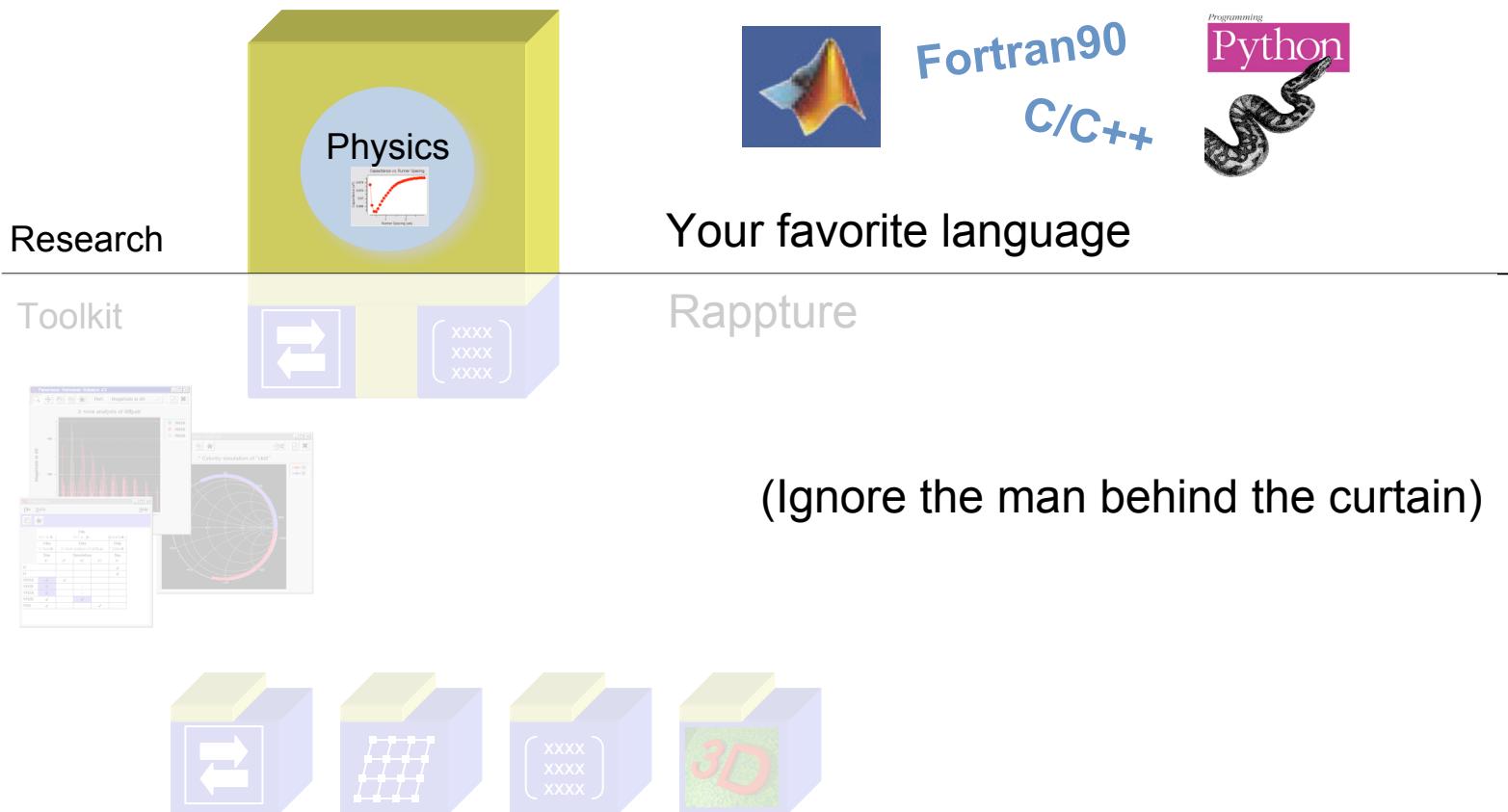
New tool in short order!

Use toolkit components,
Add unique research

Scripting language interface

Rappture toolkit components

Rappture toolkit → Rapid Application Infrastructure toolkit



Suppose you are Enrico Fermi,
and your favorite language is Python...

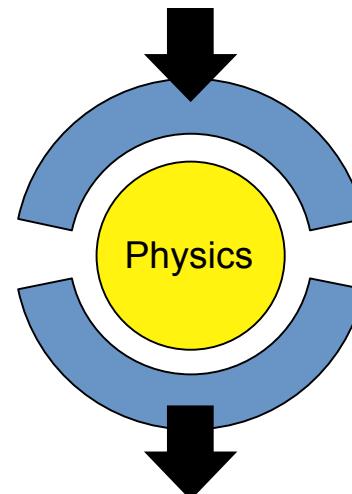
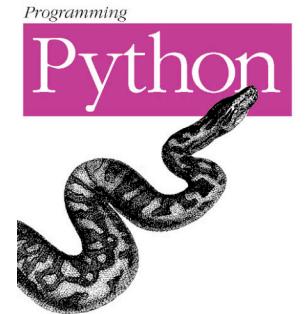
```
from math import *

T = 300 # current temperature in K
Ef = -5.5 # fermi level in eV

kT = 8.61734e-5 * T
Emin = Ef - 10*kT
Emax = Ef + 10*kT

E = Emin; dE = 0.005*(Emax-Emin)

while E < Emax:
    f = 1.0/(1.0 + exp((E - Ef)/kT))
    print 'E=%g f=%g' % (E,f)
    E += dE
```



Starting that slippery slide into I/O...

Tell Rappture about the I/O for your simulator...

```
import Rappture
```

File: fermi_io.py

```
# input parameter for temperature:  
T = Rappture.number('input.temperature',  
    label='Ambient Temperature',  
    units='K',  
    min=0, max=1000, default=300)  
  
# input parameter for Fermi level:  
Ef = Rappture.number('input.Ef',  
    label='Fermi Level',  
    units='eV',  
    default=-5.5)  
  
# table containing simulation result  
result = Rappture.table('output.result')  
result.column('Energy (eV)').units='eV'  
  
result.column('Fermi-Dirac Factor')
```

Fix your main program to use Rappture I/O...

```
from math import *
import sys
import Rappture

import fermi_io
from fermi_io import *

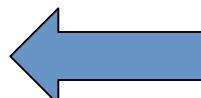
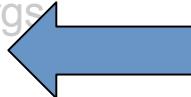
# do this right at the start, to handle command line args
Rappture.interface(sys.argv, fermi_io)
```

File: fermi.py

```
kT = 8.61734e-5 * T
Emin = Ef - 10*kT
Emax = Ef + 10*kT

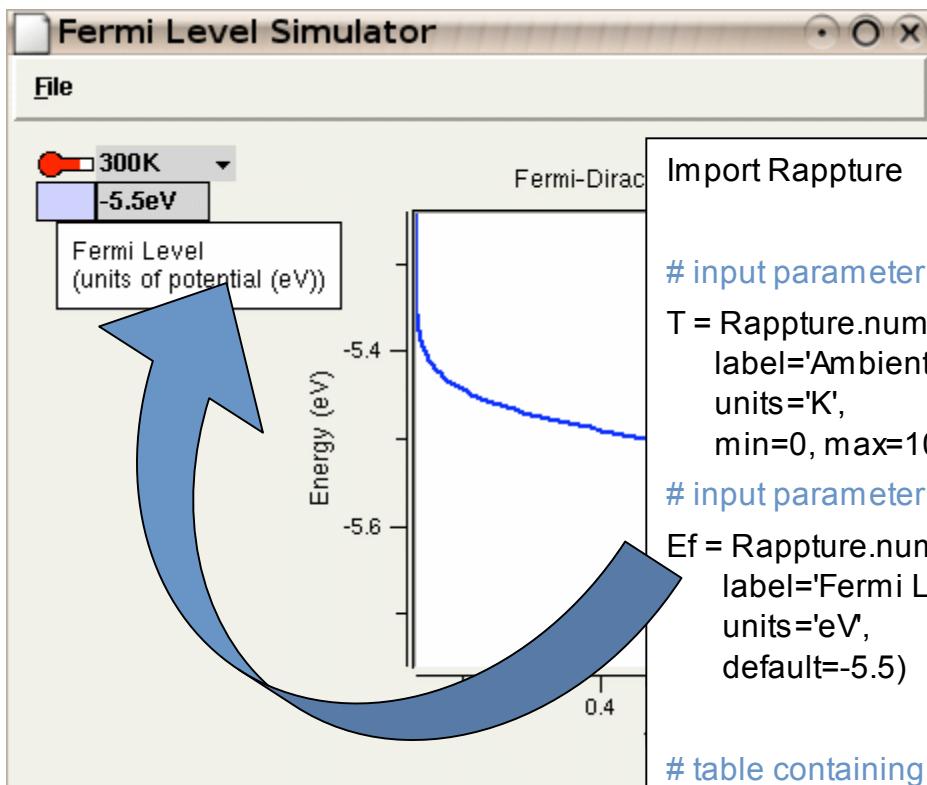
E = Emin; dE = 0.005*(Emax-Emin)
while E < Emax:
    f = 1.0/(1.0 + exp((E - Ef)/kT))
    result.append( [E,f] )
    E += dE
```

A few surgical changes



Now, run your program...

```
$ python fermi.py --gui
```



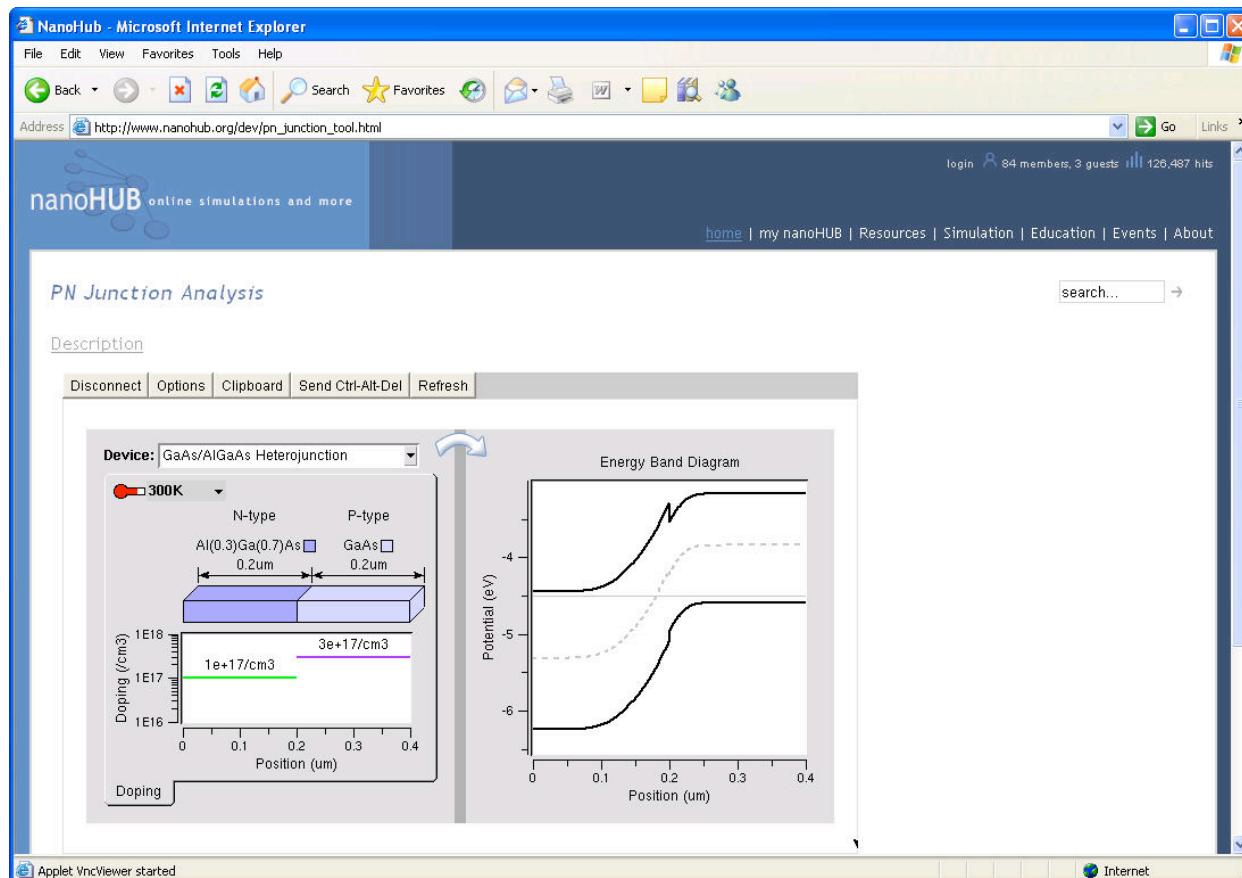
*GUI generated
automatically!*

Import Rappture

File: fermi_io.py

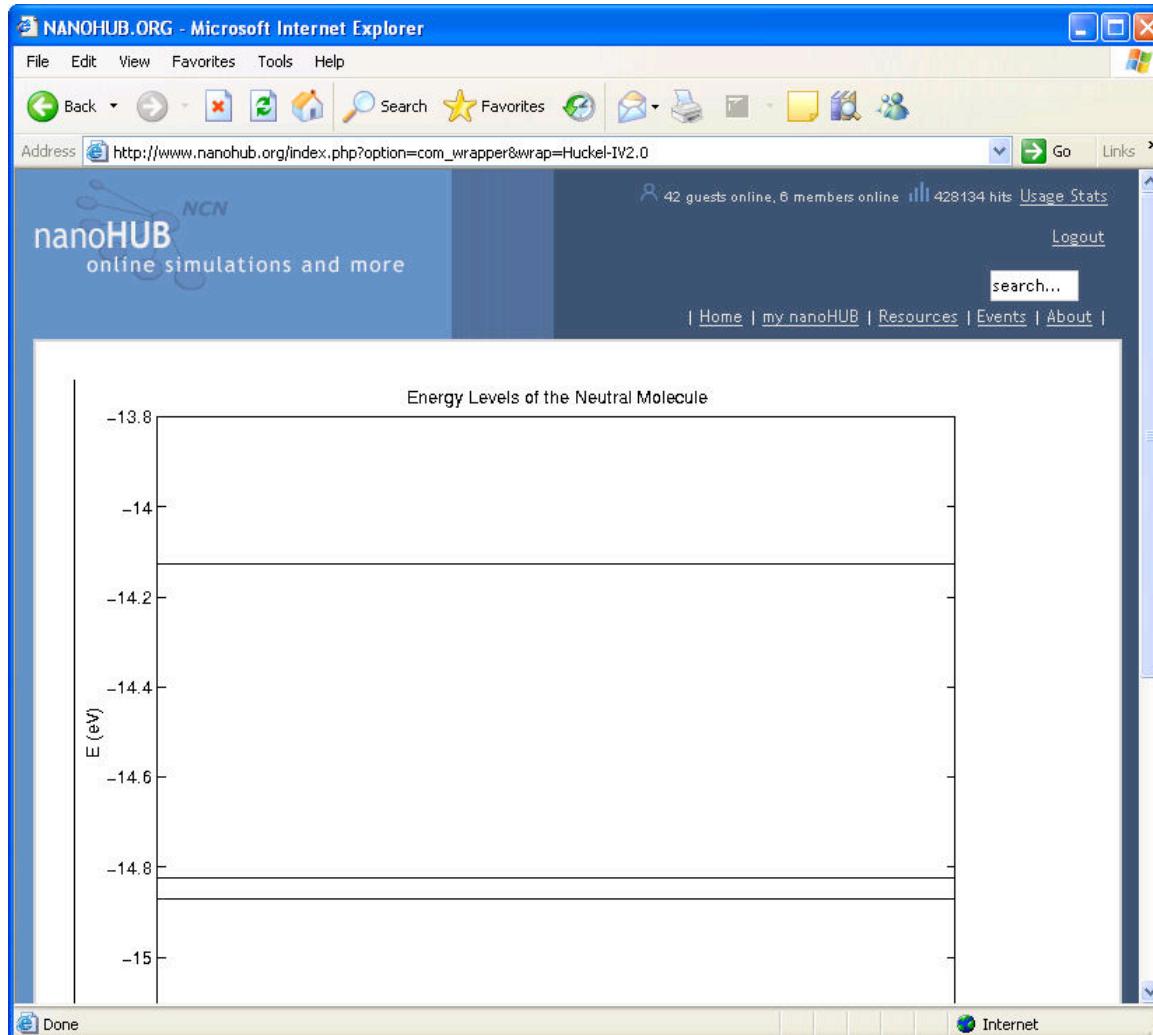
```
# input parameter for temperature:  
T = Rappture.number('input.temperature',  
    label='Ambient Temperature',  
    units='K',  
    min=0, max=1000, default=300)  
  
# input parameter for Fermi level:  
Ef = Rappture.number('input.Ef',  
    label='Fermi Level',  
    units='eV',  
    default=-5.5)  
  
# table containing output result:  
result = Rappture.table('output.result')  
result.column('Energy (eV)',units='eV')  
result.column('Fermi-Dirac Factor')
```

PN Junction Exploratory Tool

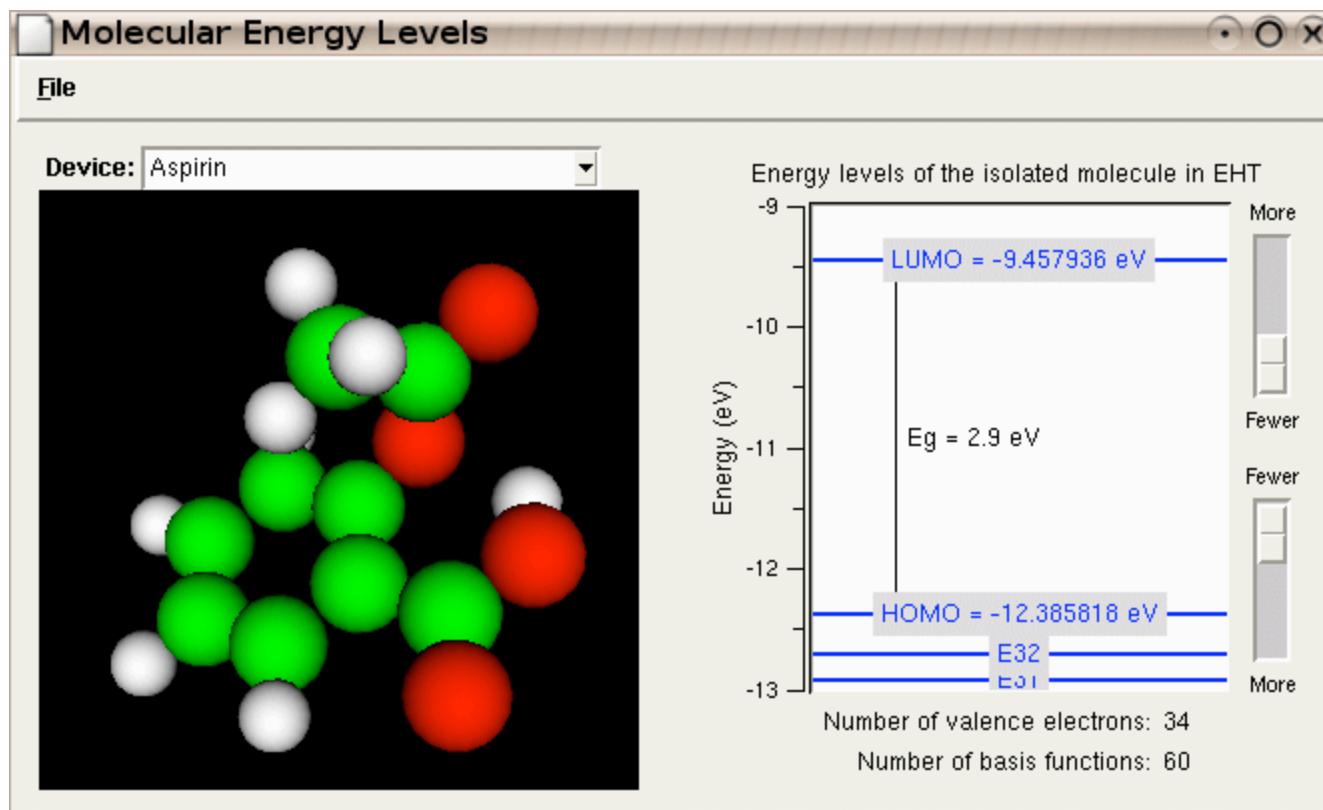


[Demo >>](#)

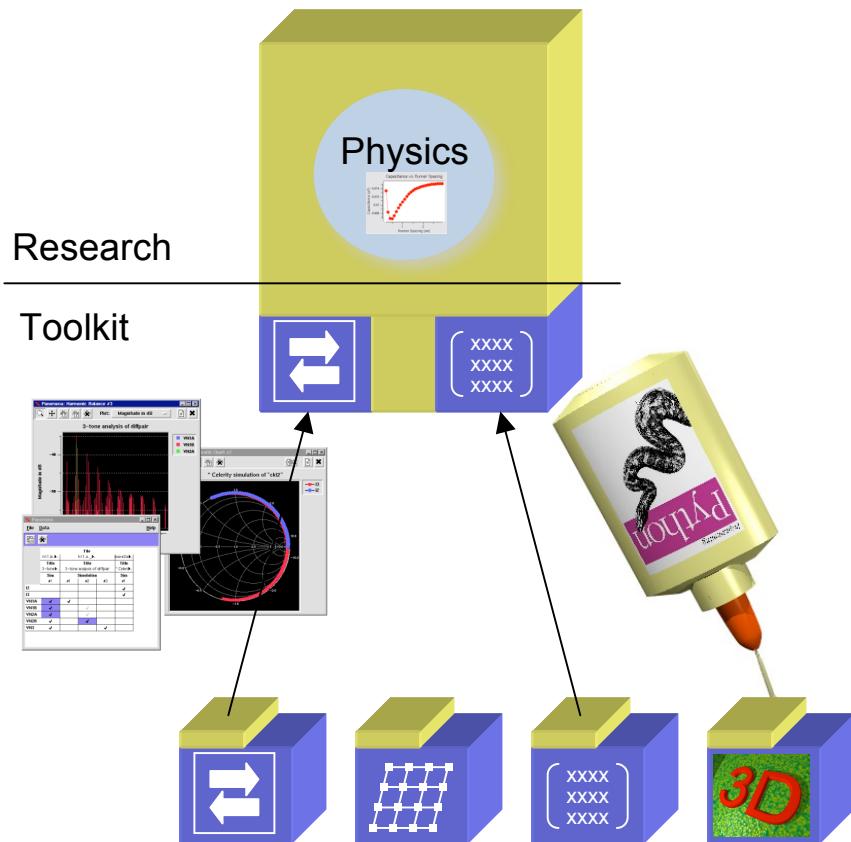
Old Version



New Version



Rappture toolkit → Rapid Application Infrastructure toolkit



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Use toolkit components,
Add unique research

Scripting language interface

Rappture toolkit components