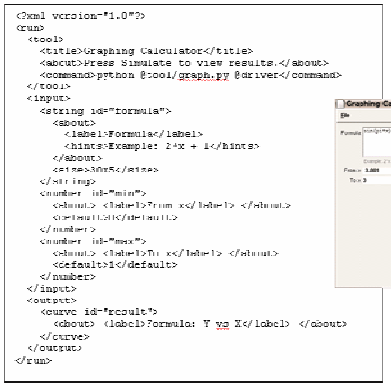
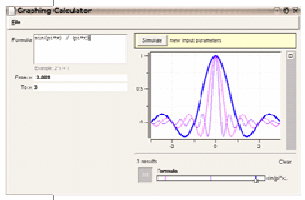
Rappture with C and Fortran



```
<?xml version="1.0"?>
<run>
  <tool>
    <title>Graphing Calculator</title>
    <about>Press Simulate to view results.</about>
    <command>python @tool/graph.py @driver</command>
  </tool>
  <input>
    <string id="formula">
      <about>
        <label>Formula</label>
        <hints>Example: 2*x + 1</hints>
      </about>
      <default>3*x^5</default>
    </string>
    <number id="min">
      <about> <label>From x</label> </about>
      <default>-3</default>
    </number>
    <number id="max">
      <about> <label>To x</label> </about>
      <default>3</default>
    </number>
  </input>
  <output>
    <curve id="result">
      <about> <label>Formula: Y vs X</label> </about>
    </curve>
  </output>
</run>
```



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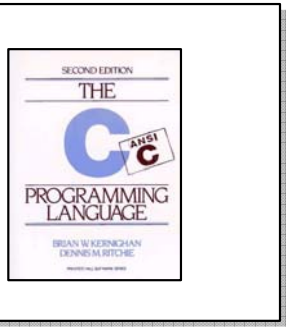
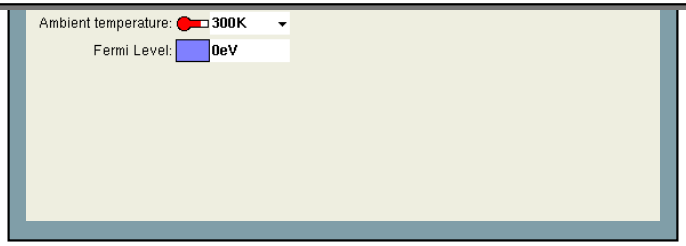
Example: app-fermi

```
<?xml version="1.0"?>
<run>
  <tool>
    <about>Press Simulate to view results.</about>
    <command>@tool/fermi @driver</command>
  </tool>
  <input>
    <number id="temperature">…</number>
    <number id="Ef">…</number>
  </input>
  <output>
    <curve id="f12">…</curve>
  </output>
</run>
```





See example code

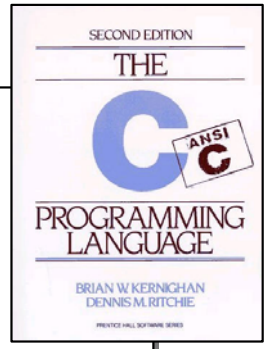
Example: app-fermi

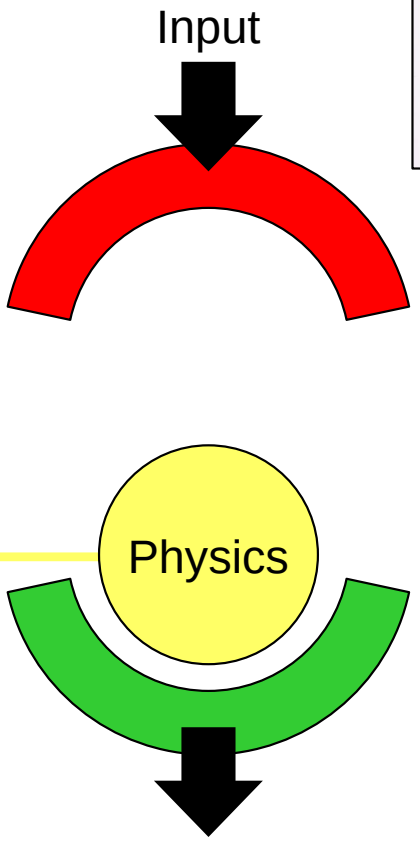
```
#include <stdio.h>
#include <math.h>
int main(int argc, char *argv[]) {
    double T, Ef, E, dE, kT, Emin, Emax, f;
    printf("Enter the Fermi energy in eV:\n");
    scanf("%lg", &Ef);
    printf("Enter the Temperature in K:\n");
    scanf("%lg", &T);
    kT = 8.61734e-5 * T;
    Emin = Ef - 10*kT;
    Emax = Ef + 10*kT;
    E = Emin;
    dE = 0.005*(Emax-Emin);
    while (E < Emax) {
        f = 1.0/(1.0 + exp((E - Ef)/kT));
        printf("%f %f\n",f, E);
        E = E + dE;
    }
    return 0;
}
```

Starting Point

fermi.c (simulator written in C)

```
#include <stdio.h>
#include <math.h>
int main(int argc, char *argv[]) {
    double T, Ef, E, dE, kT, Emin, Emax, f;
    printf("Enter the Fermi energy in eV:\n");
    scanf("%lg", &Ef);
    printf("Enter the Temperature in K:\n");
    scanf("%lg", &T);
    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));
        printf("%f %f\n",f, E);
        E = E + dE;
    }
    return 0;
}
```

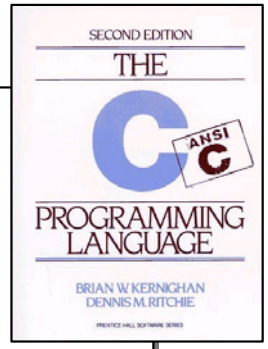


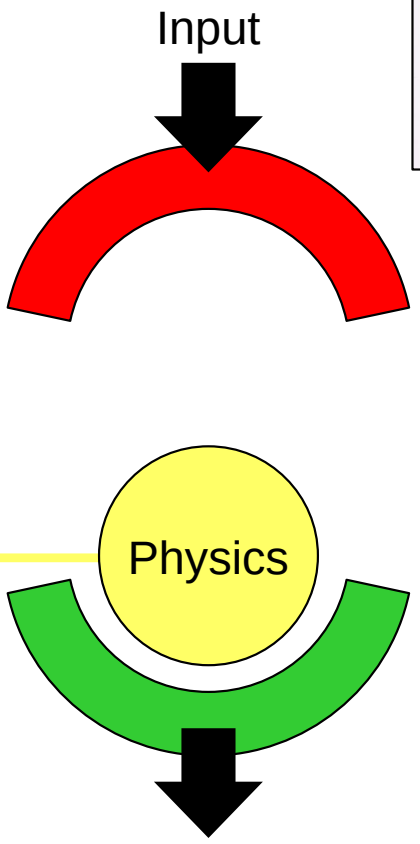


Starting Point

fermi.c (simulator written in C)

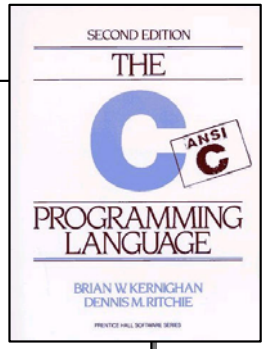
```
#include <stdio.h>
#include <math.h>
int main(int argc, char *argv[]) {
    double T, Ef, E, dE, kT, Emin, Emax, f;
    printf("Enter the Fermi energy in eV:\n");
    scanf("%lg", &Ef);
    printf("Enter the Temperature in K:\n");
    scanf("%lg", &T);
    kT = 8.61734e-5 * T;
    Emin = Ef - 10*kT;
    Emax = Ef + 10*kT;
    E = Emin;
    dE = 0.005*(Emax-Emin);
    while (E < Emax) {
        f = 1.0/(1.0 + exp((E - Ef)/kT));
        printf("%f %f\n",f, E);
        E = E + dE;
    }
    return 0;
}
```





Rappture Inputs

fermi.c (simulator written in C)



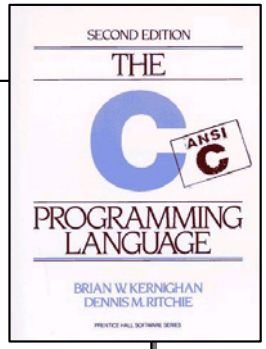

```
#include "rappture.h"
#include <stdio.h>
#include <math.h>
int main(int argc, char *argv[]) {
    double T, Ef, E, dE, kT, Emin, Emax, f; int err;
    RpLibrary *lib;
    const char* data;

    lib = rpLibrary(argv[1]);

    rpGetString(lib,"input.(temperature).current",&data);
    T = rpConvertDbl(data, "K", &err);

    rpGetString(lib,"input
    Ef = rpConvertDbl(data

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

"72F"

```
<?xml version="1.0"?>
<run>
  <tool>…</tool>
  <input>
    <number id="temperature">
      …
      <current>72F</current>
    </number>
    …
```

Rappture Inputs

fermi.c (simulator written in C)




```
#include "rappture.h"
#include <stdio.h>
#include <math.h>
int main(int argc, char *argv[]) {
    double T, Ef, E, dE, kT, Emin, Emax, f; int err;
    RpLibrary *lib;
    const char* data;

    lib = rpLibrary(argv[1]);

    rpGetString(lib,"input.(temperature).current",&data);
    T = rpConvertDbl(data, "K", &err);

    rpGetString(lib,"input.(Ef).current",&data);
    Ef = rpConvertDbl(data, "eV", &err);

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

"72F"

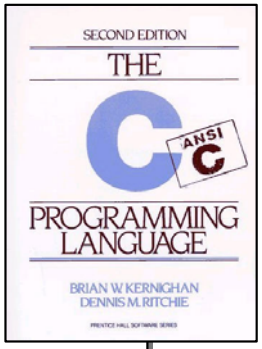
295.22

"2.4eV"

2.4

Rappture Outputs

fermi.c (simulator written in C)

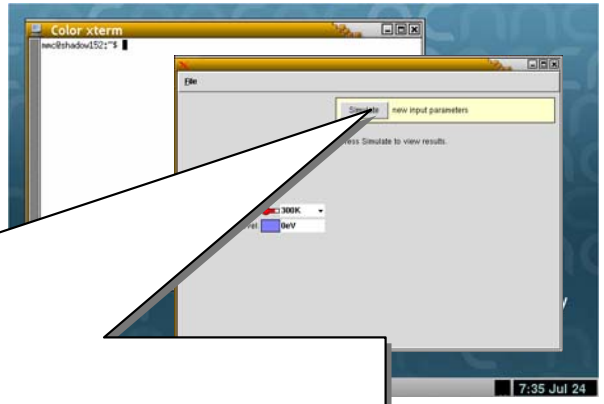



```
    …
    E = Emin;
    dE = 0.005*(Emax-Emin);
    while (E < Emax) {
        f = 1.0/(1.0 + exp((E - Ef)/kT));
        sprintf(line,"%f %f\n",f, E);      "x y \n"

        rpPutString(lib,"output.curve(f12).component.xy", line,
                    RPLIB_APPEND);

        E = E + dE;
    }

    rpResult(lib);

    return 0;
}
```

```
<?xml version="1.0"?>
<run>
  <tool>…</tool>
  <input>…</input>
  <output>
    <curve id="f12">
      <component><xy>0.999955 -0.25852
0.99995 -0.255935 …
```

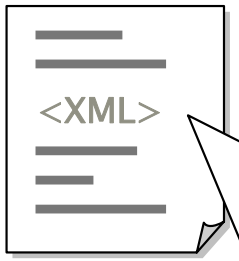
Compiling the Rappturized Code

From your workspace...




```
% cd tooldir
% ls
tool.xml fermi.c

% gcc -g fermi.c –o fermi –I/apps/rappture/current/include
–L/apps/rappture/current/lib –lrappture -lm
% ls
tool.xml fermi.c fermi

% rappture
```

How does the program get invoked?



tool.xml

Replaced with directory containing tool.xml file
Ex: `/apps/yourtool/current`

Replaced with name of driver file
Ex: `driver327.xml`

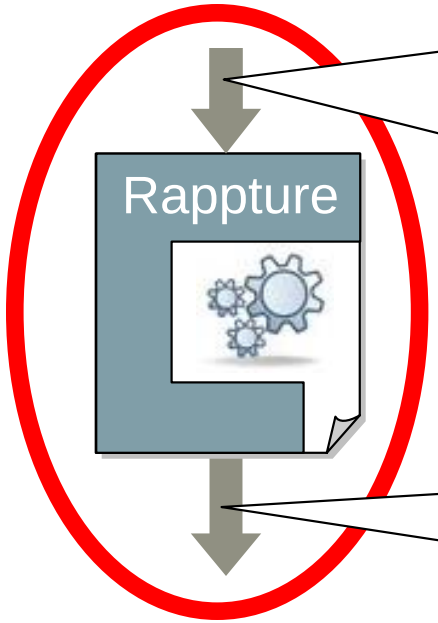
```
<?xml version="1.0"?>
<run>
  <tool>
    <about>Press Simulate to view results.</about>
    <command>@tool/fermi @driver </command>
  </tool>
  <input>
    …
  </input>
  <output>
    …
  </output>
</run>
```

…with the driver file as the first argument

Invoke the C program…

How does the program get invoked?

```
@tool/fermi @driver
/apps/yourtool/current/fermi driver327.xml
```




```
#include "rappture.h"
…
int main(int argc, char *argv[]) {
    double T, Ef, E, dE, kT, Emin, Emax, f;
    RpLibrary *lib;
    const char* data;
    lib = rpLibrary(argv[1]);
…
```

```
…
    rpResult(lib);
    return 0;
}
```

Not Much Overhead

It's easy to add Rappture to your new tools:

Instead of this…

Documentation

```
scanf("%lg",&Ef);
```

```
printf("%g",Ef);
```

Do this…

```
<number id="Ef">
  <about>
    <label>Fermi Level</label>
  </about>
  <units>eV</units>
  <default>0eV</default>
</number>
```

```
rpGetString(lib, path, &data);
Ef = rpConvertDbl(data, "eV", &err);
```

```
rpPutString(lib, path, val, RPLIB_APPEND);
…
rpResult(lib);
```

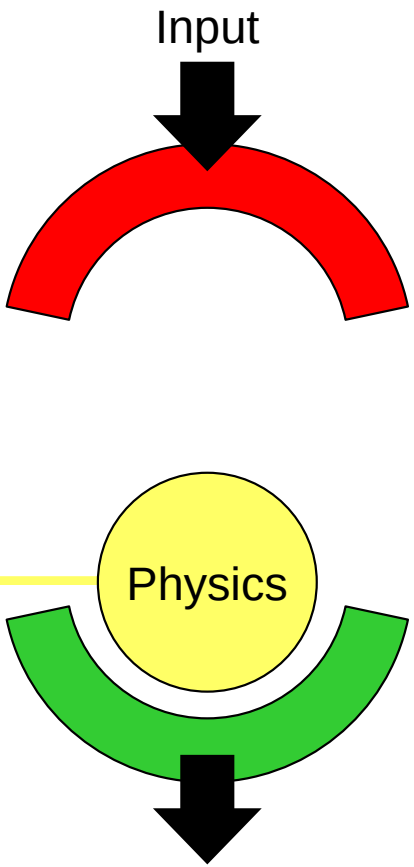
Example: app-fermi

```
      program fermi

        read(5,*) Ef
        read(5,*) T

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

        dE = 0.005*(Emax - Emin)

        do 10 E=Emin,Emax,dE
          f = 1.0/(1.0+exp((E-Ef)/kT))

          write(6,*) f, E

10      continue

      end program fermi
```

Starting Point

fermi.f (simulator written in Fortran)

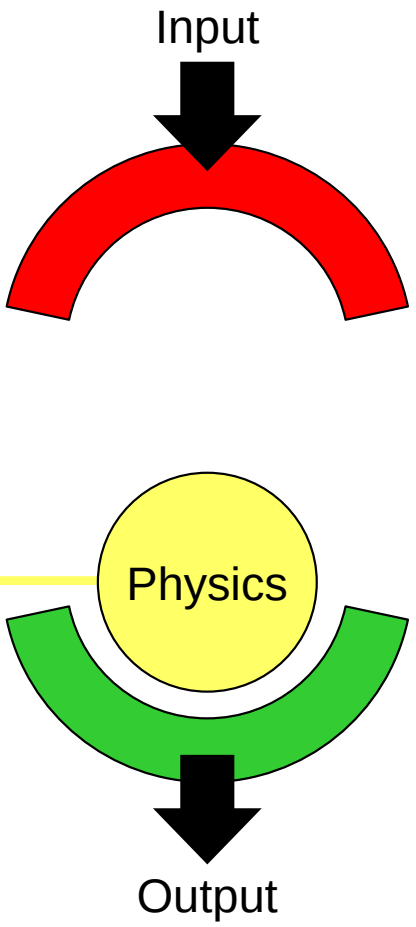
```
      program fermi

       read(5,*) Ef
       read(5,*) T

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

        dE = 0.005*(Emax - Emin)

       do 10 E=Emin,Emax,dE
         f = 1.0/(1.0+exp((E-Ef)/kT))

         write(6,*) f, E

10      continue

      end program fermi
```



Starting Point

fermi.f (simulator written in Fortran)

```
      program fermi

       read(5,*) Ef
       read(5,*) T

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

        dE = 0.005*(Emax - Emin)

       do 10 E=Emin,Emax,dE
         f = 1.0/(1.0+exp((E-Ef)/kT))

         write(6,*) f, E

10      continue

      end program fermi
```



Fortran F77

Rappture Inputs

fermi.f (simulator written in Fortran)


```
      program fermi

      call getarg(1,inFile)
      driver = rp_lib(inFile)

      call rp_lib_get(driver,
     +       "input.number(temperature).current", str)

      okay = rp_units_convert_dbl(str, "K", T)

      call rp_lib_get(driver,
     +       "input.number(Ef).current", str)

      okay = rp_units_convert_dbl(str, "eV", Ef)

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

      dE = 0.005*(Emax - Emin)
...
```

"72F"

295.22

"2.4eV"

2.4

Rappture Outputs

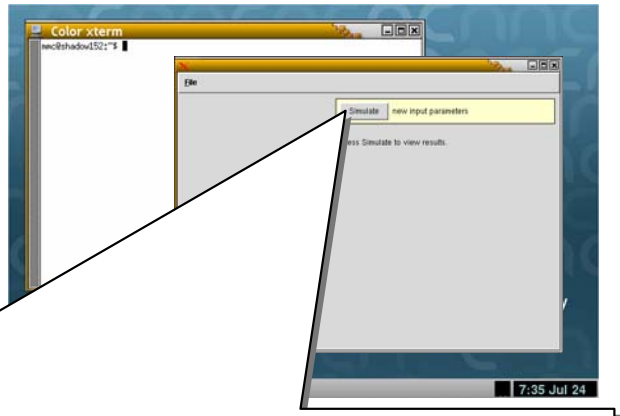
fermi.f (simulator written in Fortran)


```
        …
        dE = 0.005*(Emax - Emin)

        do 10 E=Emin,Emax,dE
          f = 1.0/(1.0+exp((E-Ef)/kT))

          write(xy,'(E20.12, F13.9, A)') f, E, char(10)

          call rp_lib_put_str(driver,
     +         "output.curve(f12).component.xy", xy, 1)

10      continue

        call rp_result(driver)

      end program fermi
```

"x y \n"

Compiling the Rappturized Code

From your workspace...




```
% cd tooldir
% ls
tool.xml fermi.f

% g77 -g fermi.f –o fermi –L/apps/rappture/current/lib –lrappture
% ls
tool.xml fermi.f fermi

% rappture
```

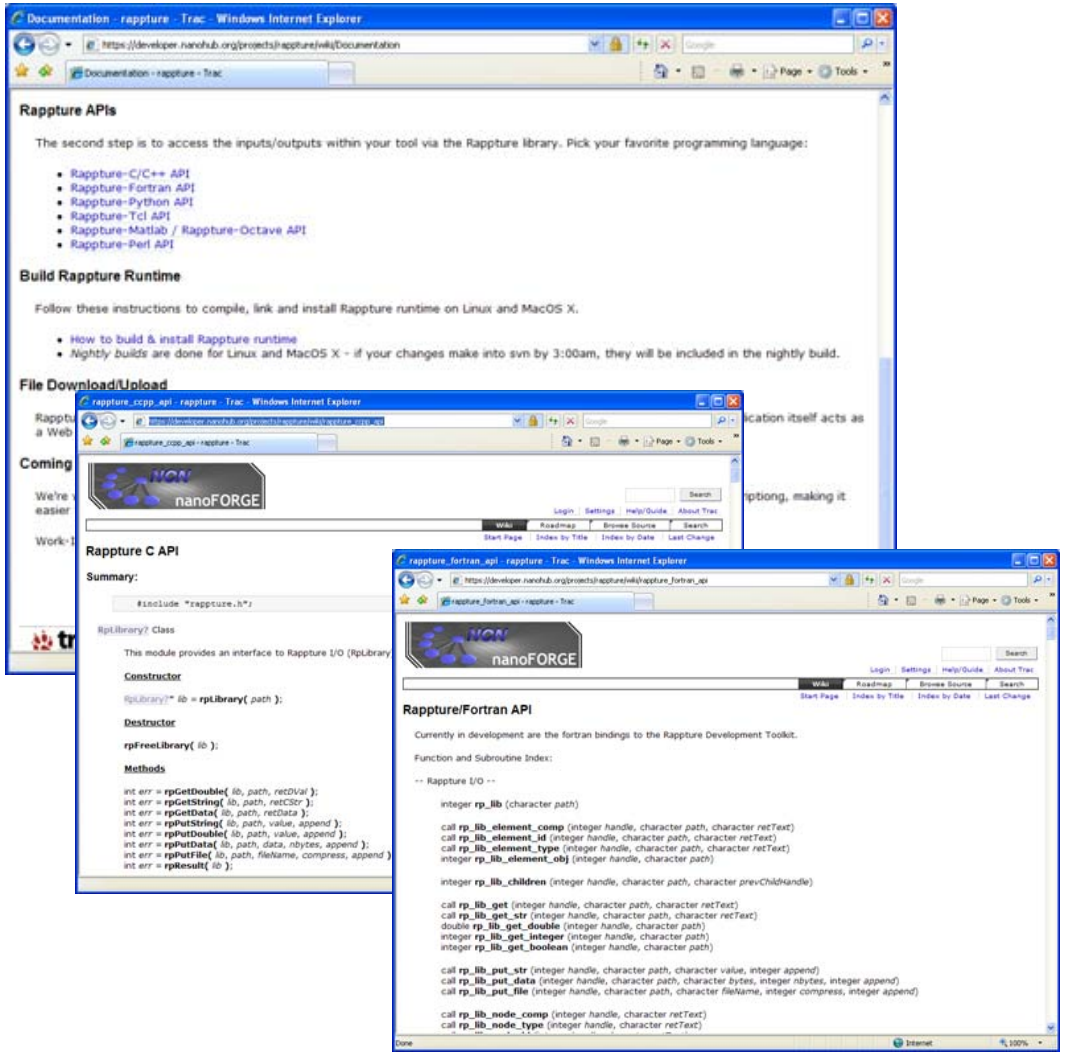
Reference Documentation

http://rappture.org

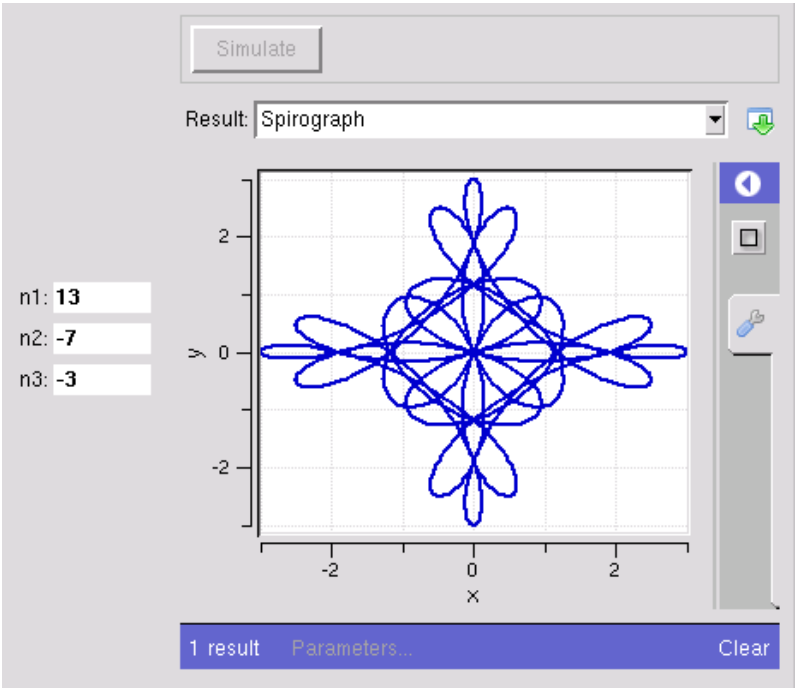
- Documentation
- Rappture-C/C++ API
- Rappture-Fortran API

Examples:

- app-fermi in C
- app-fermi in Fortran



Exercise #3: Build a Spirograph Program



Try these values:

$n_1 = 13$	$n_1 = 19$	$n_1 = 7$
$n_2 = -7$	$n_2 = -13$	$n_2 = -5$
$n_3 = -3$	$n_3 = 3$	$n_3 = 2$

Download assignment:
http://hubzero.org/resources/160 ex3.zip

```
#include <stdio.h>
#include <math.h>
#include <complex.h>

int
main(int argc, char **argv)
{
    double n1, n2, n3, t;
    double complex z;

    printf("Enter value: n1 = ");  scanf("%lg", &n1)
    printf("Enter value: n2 = ");  scanf("%lg", &n2)
    printf("Enter value: n3 = ");  scanf("%lg", &n3)

    for (t=0.0; t < 1.0; t += 0.001) {
        z = cexp(I*2*M_PI*n1*t) + cexp(I*2*M_PI*n2*t
        printf("%g %g\n", creal(z), cimag(z));
    }

    return 0;
}
```