PYTHON VIRTUAL ATOMIC FORCE MICROSCOPE (PYVAFM)

MAINZ TUTORIAL 2015

CONTENTS

- Brief introduction to the PyVAFM (15mins)
- Hands on tutorial
  - FM-AFM simulation (1hr15mins)

```
#!/usr/bin/env python
import sys
sys.path.append('/home/vafm/src')
from vafmcircuits import Machine
from customs import *
import sys

#Force Field units are nm and nN
#Variables
f0=
Az= #nm
Q=
k= #N/m


#Adding Circuits Section 1
##############################
machine = Machine(machine=None, name
scanner = machine.AddCircuit(type='S

inter = machine.AddCircuit(type='i3D
inter.Configure(steps=[0.0508,0.0616
inter.Configure(pbc=[True,True,False
inter.Configure(ForceMultiplier=0.00
inter.ReadData('ForceField.dat')

canti = machine.AddCircuit(type='Can

machine.AddCircuit(type="Machine",na


##############################
#Add PI Circuit Here
```

ATOMIC FORCE MICROSCOPY

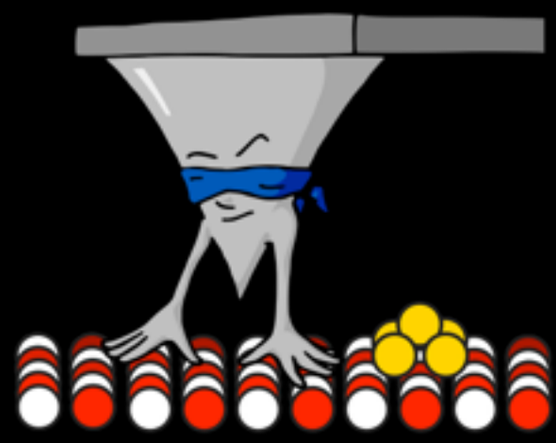
- Cantilever is oscillated above the surface
- The cantilever feels interactions from the surface and surrounding medium
- These Interactions shift the resonance frequency of the cantilever

AM-AFM

- The driving signal of the cantilever is kept constant.
- Hence when the resonance frequency of the cantilever shifts the amplitude will change.
- Simpler to setup but can’t be rarely used in vacuum due to the large Q factor of the system

FM-AFM

- Directly uses shift in frequency for contrast
- More complicated to set up since it requires several feedback loops
- Can be operated in any environment.



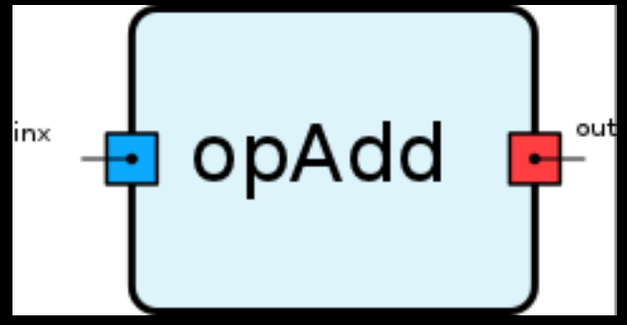
WHAT IS THE PYVAFM?

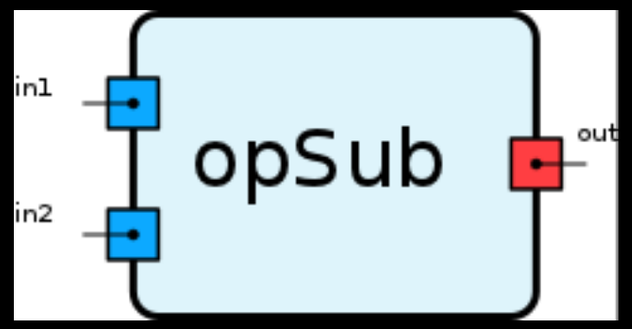
- Atomic Force Microscope simulator
- Allows users to reproduce experimental images
    - Hence allowing such things as contrast mechanisms to be identified
- Capable of recreating any experimental mode or parameters.

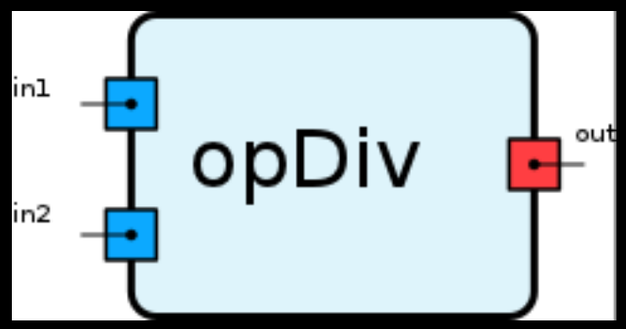
```
scanner = machine.AddCircuit(type='Scanner',name='scan', Process = m

inter = machine.AddCircuit(type='i3Dlin',name='inter', components=1,
inter.Configure(steps=[0.0508,0.0616625,0.005], npoints=[16,8,200])
inter.Configure(pbc=[True,True,False])
inter.Configure(ForceMultiplier=0.00166) # the values here are KJ/mo
inter.ReadData('ForceField.dat')
```

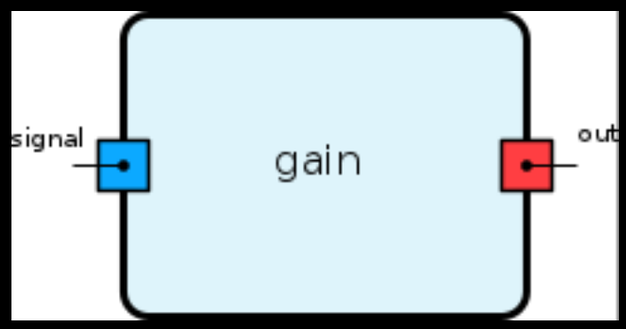
MODULARITY

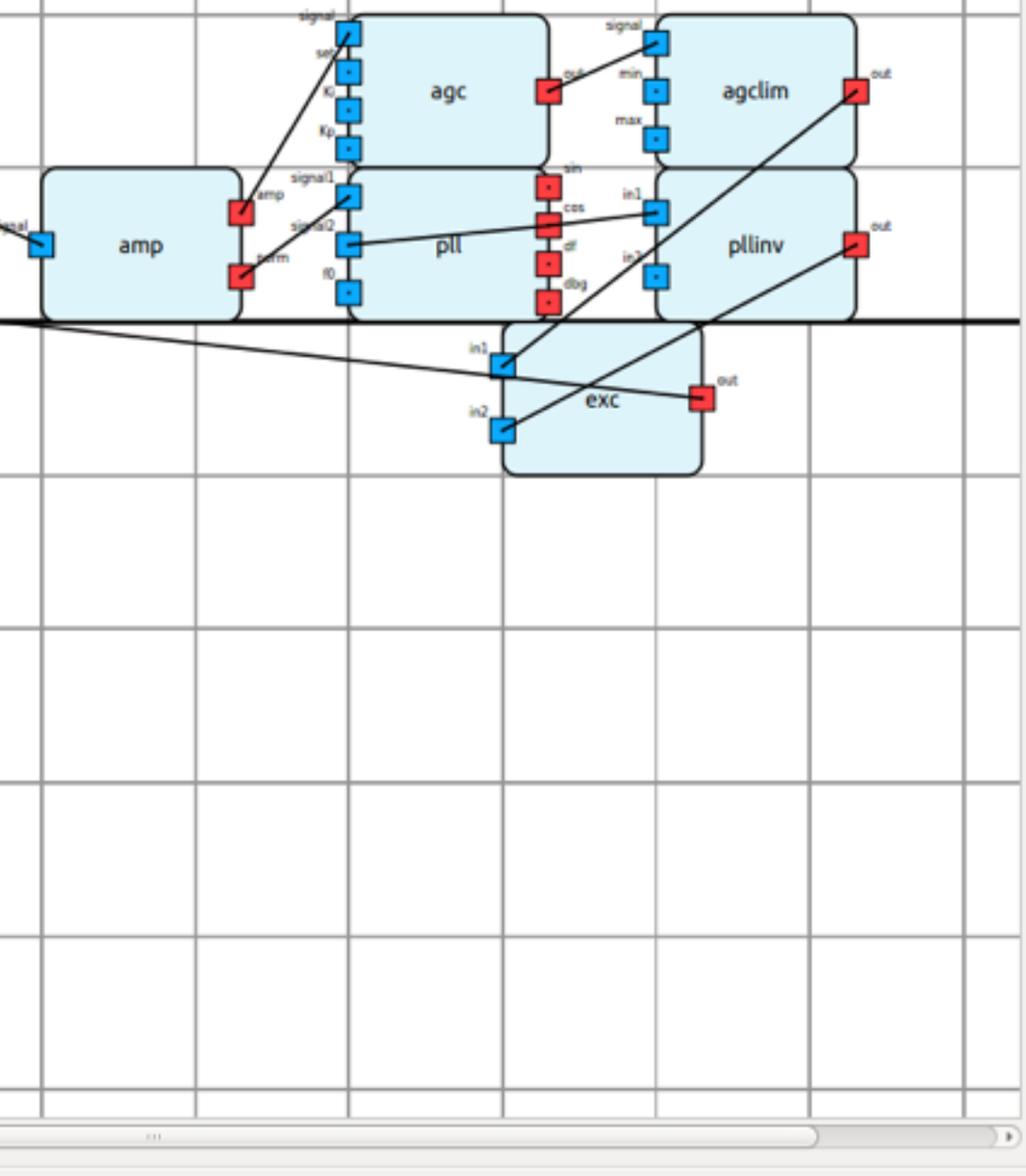
- A modular simulation allows any experimental setup to be reproduced.
- Each module is referred to as a circuit











CIRCUITS

- Black boxes that simulate real life processes:
  - Such as a low pass filter.
- Circuits contain Input and Output channels:
  - Allowing them to be connected together.
- Hence you can build any simulation setup by connecting the circuits in various ways! http://www.electronic-circuits-diagrams.com/wp-content/uploads/2014/08/210.gif
- Possible to add your own custom circuits

DOCUMENTATION

- http://singroup.github.io/PyVAFM/
- Contains information on how to use every circuit.
- Also contains additional tutorials and information regarding the PyVAFM.

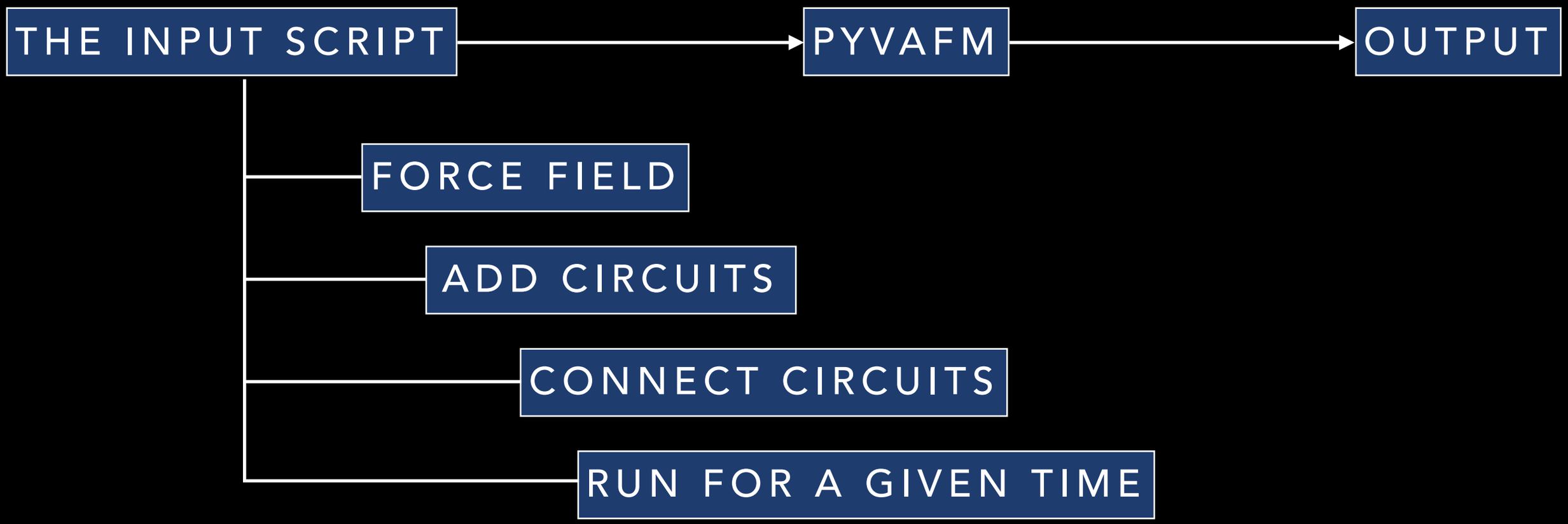
Pythonic Virtual Machine

pyVAFM Documentation

Welcome to the pyVAFM documentation.

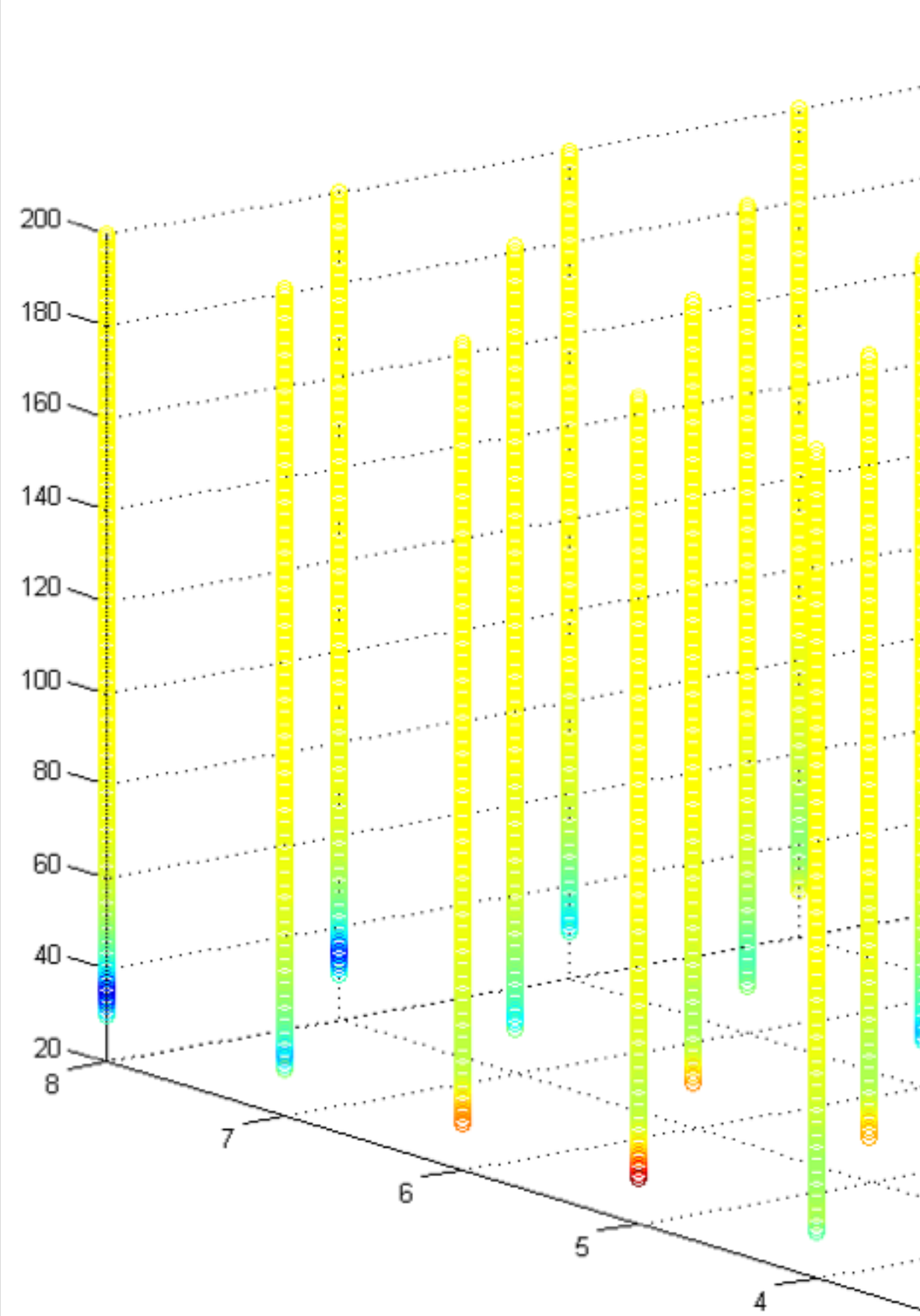
1. Installation
    a. Prerequisites
    b. Installation
    c. Running
2. Quick Start
3. User Manual
    a. Circuits

ANATOMY OF A SIMULATION



FORCE FIELD

- A 3d field describing the interactions the tip feels above a surface.
- The units of the vAFM is defined by the force field.
- Force fields are usually obtained from external calculations i.e. Molecular Dynamics simulations.



INPUT SCRIPT

- The input scripts is where you add and connect all your circuits.

- Input scripts are written in python.

- Although you can get by without extensive python knowledge.

```
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##########################
#Add PI Circuit Here
```

ADDING CIRCUITS

Circuits must be added to the simulation before they can be used.

Circuits are updated in the order you add them

When adding a circuit you must specify :

The type of circuit you want to add

Unique name of the circuit

Initialisation paramaters

Push the circuit?

```
18    machine.AddCircuit(type='waver',name='osc', amp=1, freq=1e4, pushed=True)
```

```
17    inter = machine.AddCircuit(type='i3Dlin',name='inter', components=3, pushed=True)
18
19    inter.Configure(steps=[0.705,0.705,0.1], npoints=[8,8,171])
20    inter.Configure(pbc=[True,True,False])
21    #inter.Configure(ForceMultiplier=1e10)
22    inter.ReadData('NaClforces.dat')
```

Additional Setup

```
29    #Outputs
30    out1 = machine.AddCircuit(type='output',name='output',file='interpolationtest.dat', dump=1)
31    out1.Register('global.time', "scann.x","scann.y","scann.z",'inter.F1')
```

CONNECTING CIRCUITS

In order for circuits to communicate they must be connected

Outputting circuit name, this was defined when adding the circuit

Circuits output channel

```
23      machine.Connect("osc.cos","pll.signal1")
```

Input circuit name, this was defined when adding the circuit

Circuit output channel

Connects circuit named “osc” without an output channel called “cos” to a circuit named “pll” with a input channel called “signal1”

RUNNING THE SIMULATION

vAFM integrates over time.

We can either run the vAFM for a given amount of time..

```
30      machine.Wait(0.01)
```

or move the tip around

```
89      scanner.Place(x=0,y=0,z=15)
90      scanner.Move(x=0,y=0,z=-1)
```

Hands on Tutorial

This brief presentation has introduced you to the basic ideas of the PyVAFM

Some setup details have been left out for a more compete tutorial please visit http://singroup.github.io/PyVAFM/

In order to speed things up an input script has already been mostly prepared for you.

Your task is to:

Add and connect an amplitude detection system and tune it.

Add and connect Phase Locked Loop and tune it.

Script the Cantilever

Get an image