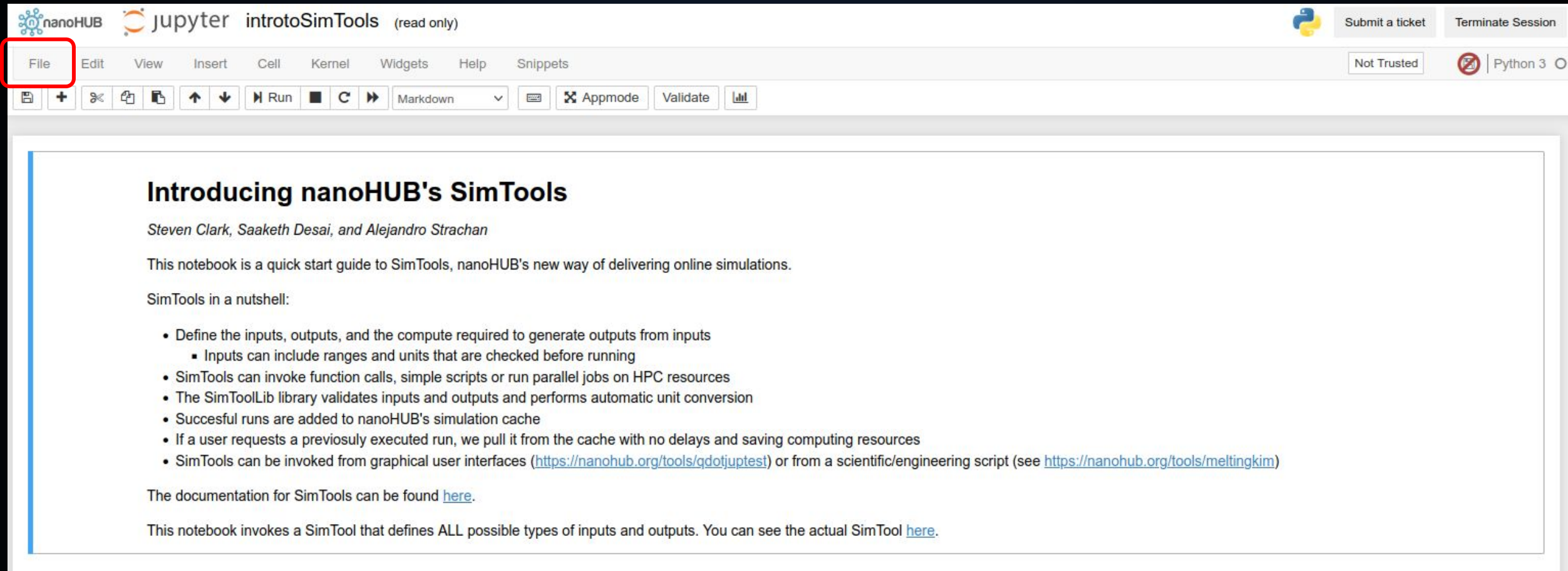


Sim2Ls: Software tools that are FAIR

1. Introduction to Sim2Ls - Motivation
2. Introduction to nanoHUB notebooks
3. Sim2Ls organization/structure
4. Build a Sim2L - pendulum motion
5. HUBzero integration
6. Questions/Discussion

introSimTools - workflow notebook



The screenshot shows the nanoHUB Jupyter interface. At the top, the nanoHUB logo is on the left, and the text "jupyter introSimTools (read only)" is in the center. On the right, there are links for "Submit a ticket" and "Terminate Session". Below this is a menu bar with "File", "Edit", "View", "Insert", "Cell", "Kernel", "Widgets", "Help", and "Snippets". The "File" menu is highlighted with a red box. Below the menu bar is a toolbar with icons for saving, opening, and running files, as well as buttons for "Appmode", "Validate", and a chart icon. The main content area displays the notebook text.

Introducing nanoHUB's SimTools

Steven Clark, Saaketh Desai, and Alejandro Strachan

This notebook is a quick start guide to SimTools, nanoHUB's new way of delivering online simulations.



SimTools in a nutshell:

- Define the inputs, outputs, and the compute required to generate outputs from inputs
 - Inputs can include ranges and units that are checked before running
- SimTools can invoke function calls, simple scripts or run parallel jobs on HPC resources
- The SimToolLib library validates inputs and outputs and performs automatic unit conversion
- Successful runs are added to nanoHUB's simulation cache
- If a user requests a previously executed run, we pull it from the cache with no delays and saving computing resources
- SimTools can be invoked from graphical user interfaces (<https://nanohub.org/tools/qdotjuptest>) or from a scientific/engineering script (see <https://nanohub.org/tools/meltingkim>)

The documentation for SimTools can be found [here](#).

This notebook invokes a SimTool that defines ALL possible types of inputs and outputs. You can see the actual SimTool [here](#).

introtoolsimtools - file explorer



 



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<input type="checkbox"/>	doc		7 minutes ago	
<input type="checkbox"/>	examples		7 minutes ago	
<input type="checkbox"/>	middleware		7 minutes ago	
<input type="checkbox"/>	simtool		7 minutes ago	
<input type="checkbox"/>	src		7 minutes ago	
<input type="checkbox"/>	 introtoSimTools.ipynb	Running	7 minutes ago	47 B
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<input type="checkbox"/> 0 ▾	/ simtool	Name ▾	Last Modified	File size
<input type="checkbox"/>	..		seconds ago	
<input type="checkbox"/>	 introtoolsimtools.ipynb		10 minutes ago	55 B

introtoolsimtools - sim2L notebook

Introducing nanoHUB's SimTools

Steven Clark, Saaketh Desai, and Alejandro Strachan

This notebook is a quick start guide to SimTools, nanoHUB new way of delivering online simulations.

SimTools in a nutshell

- Define the inputs, outputs, and the compute required to generate outputs from inputs
 - Inputs can include ranges and units that are checked before running
- SimTools can invoke parallel jobs running on HPC resources, a simple script, or evaluating a function call
- The SimToolLib library validates inputs and outputs, including automatic unit conversion
- Successful runs are added to nanoHUB's simulation cache
- If a user requests a previously executed run, we pull it from the cache with no delays and saving computing resources
- SimTools can be invoked from graphical user interfaces (example here) or from a scientific/engineering script (example here)

The documentation for SimTools can be found [here](#).

This notebook demonstrates a simple SimTools that demonstrates all the possible input and output types.

Step 1. Provide a description of your tool

This cell is optional but highly recommended. The provided description is displayed when returning SimTool search results.

In []:

DESCRIPTION ✕

```
DESCRIPTION = """Show examples of SimTool input and output types"""
```


introtosimtools - sim2L notebook

In []:

```
%load_ext yamlmagic
```

Step 2. Define all inputs. Including valid ranges and units is strongly encouraged

In []:

```
%%yaml INPUTS
```

```
booleanValue:  
  type: Boolean  
  description: Execute bogus save operations  
  value: False
```

```
textString:  
  type: Text  
  description: Text supplied as string  
  value: textString
```

```
textFile:  
  type: Text  
  description: Text supplied as file
```

```
integerValue:  
  type: Integer  
  description: Simple integer  
  value: 10
```

```
numberValue:  
  type: Number  
  description: Simple number  
  value: 10.5  
  min: 0.0  
  max: 100.0  
  units: K
```

```
# Specifying units clearly defines the units that the SimTool expects for the input.  
# Examples of inputs are K (for temperature), angstroms (for distance) and fs for time.  
# If the input from the user is in some other units, we use the Pint library (https://pint.readthedocs.io/en/0.10.1/)  
# to automatically convert the units, and, in combination with range checking, validating inputs for all SimTool runs.  
# See the pint documentation for a list of allowable units.
```

introtoolsimtools - sim2L notebook

In []:

FILES ✕

```
# If you simulation require additional files (e.g. configuration files), list them here. The files  
# should exist in the same directory (simtool) as this notebook.  
# This cell is optional. The tag FILES and variable EXTRA_FILES must specified exactly as given here.  
EXTRA_FILES = []
```

In []:

parameters ✕

```
from simtool import getValidatedInputs  
  
defaultInputs = getValidatedInputs(INPUTS)  
if defaultInputs:  
    globals().update(defaultInputs)
```

introtosimtools - sim2L notebook

In []:

```
%%yaml OUTPUTS
```

```
booleanValue:
```

```
  type: Boolean
```

```
  description: Execute bogus save operations
```

```
  value: False
```

```
textString:
```

```
  type: Text
```

```
  description: Text supplied as string
```

```
  value: textString
```

```
textFile:
```

```
  type: Text
```

```
  description: Text supplied as file
```

```
integerValue:
```

```
  type: Integer
```

```
  description: Simple integer
```

```
  value: 10
```

```
numberValue:
```

```
  type: Number
```

```
  description: Simple number
```

```
  value: 10.5
```

```
  min: 0.
```

```
  max: 100.
```

```
arrayValue:
```

```
  type: Array
```

```
  description: Array of numbers
```

```
  value: [1,2,3]
```

intro simtools - sim2L notebook

In []:

```
db = DB(OUTPUTS)
```

In []:

```
print(booleanValue)
db.save('booleanValue', booleanValue)

print(integerValue)
db.save('integerValue', integerValue)

print(numberValue)
db.save('numberValue', numberValue)

print(textString)
db.save('textString', textString)

print(textFile)
copyAndSaveFileAsOutput('textFile', textFile)

print(imageFile)
copyAndSaveFileAsOutput('imageFile', imageFile)

print(imageValue)
db.save('imageValue', imageValue)

print(arrayValue)
db.save('arrayValue', arrayValue)

print(arrayFile)
copyAndSaveFileAsOutput('arrayFile', arrayFile)

print(listValue)
db.save('listValue', listValue)

print(listFile)
copyAndSaveFileAsOutput('listFile', listFile)

print(dictValue)
db.save('dictValue', dictValue)
```


introtools - sim2L notebook

```
print(dictValue)
db.save('dictValue', dictValue)

print(dictFile)
copyAndSaveFileAsOutput('dictFile', dictFile)

print(choiceValue)
db.save('choiceValue', choiceValue)

print(elementValue)
db.save('elementValue', elementValue)
```

False

10

10.5

textString

None

None

None

[1, 2, 3]

None

['one', 'two', 'three']

None

{'one': 1, 'two': 2, 'three': 3}

None

pear

58.6934

introtoolsimtools - workflow notebook

Step 1. Setting things up

```
In [1]: # We will import various libraries including key elements of nanoHUB's simtool library
        %load_ext yamlmagic

        import os
        import numpy as np
        import PIL.Image

        from simtool import findInstalledSimToolNotebooks, searchForSimTool
        from simtool import getSimToolInputs, getSimToolOutputs, Run

In [2]: # Identify the simtool of interest (in this case introducing simtools) and retrieve its status
        simToolName = "introtoolsimtools"
        simToolLocation = searchForSimTool('introtoolsimtools')
        for key in simToolLocation.keys():
            print("%18s = %s" % (key, simToolLocation[key]))

        notebookPath = /apps/introtoolsimtools/r13/simtool/introtoolsimtools.ipynb
        simToolName = introtoolsimtools
        simToolRevision = r13
        published = True
```

introtosimtools - workflow notebook

Step 2. Inputs

```
In [3]: # get the list of inputs for the simtool. This is an exhaustive list of inputs for SimTools.  
inputs = getSimToolInputs(simToolLocation)  
inputs
```

```
integerValue:  
  min: None  
  max: None  
  type: Integer  
  description: Simple integer  
  value: 10
```

```
numberValue:  
  units: kelvin  
  min: 0.0  
  max: 100.0  
  type: Number  
  description: Simple number  
  value: 10.5
```

```
arrayValue:  
  min: None  
  max: None  
  type: Array
```

introtosimtools - workflow notebook

```
In [4]: inputs['booleanValue'].value = False
inputs['integerValue'].value = 5
inputs['numberValue'].value = 10.7
inputs['textString'].value = "Now is the time for all good men to come to the aid of their party"
inputs['textFile'].file = os.path.join("data", "Text", "party.txt")
inputs['imageFile'].file = os.path.join("data", "Images", "dome_qd_simple.png")
inputs['imageValue'].value = PIL.Image.open(os.path.join("data", "Images", "jup.png"))
inputs['arrayValue'].value = np.array([[1., 2., 3.], [4., 5., 6.], [7., 8., 9.]])
inputs['arrayFile'].file = os.path.join("data", "Array", "2Darray.json")
inputs['listValue'].value = ['one', 'two', 'three', 'seven']
inputs['listFile'].file = os.path.join("data", "List", "list.json")
inputs['dictValue'].value = {'one': 2, 'two': 2, 'three': 3}
inputs['dictFile'].file = os.path.join("data", "Dict", "dict.json")
inputs['choiceValue'].value = "apple"
inputs['elementValue'].value = "Fe"

inputs
```

```
integerValue:
  min: None
  max: None
  type: Integer
  description: Simple integer
  value: 5
```

```
numberValue:
  units: kelvin
  min: 0.0
  max: 100.0
  type: Number
  description: Simple number
  value: 10.7
```

```
arrayValue:
  min: None
  max: None
  type: Array
```

introSimtools - workflow notebook

```
In [5]: # We can explore the outputs the SimTool will produce before running the simulation.  
# Of course, at this point all output variables are empty  
outputs = getSimToolOutputs(simToolLocation)  
outputs
```

```
Out[5]: booleanValue:  
    type: Boolean  
    description: Execute bogus save operations  
    value: False  
  
    textString:  
        type: Text  
        description: Text supplied as string  
        value: textString  
  
    textFile:  
        type: Text  
        description: Text supplied as file  
  
    integerValue:  
        min: None  
        max: None  
        type: Integer  
        description: Simple integer  
        value: 10
```


introtosimtools - workflow notebook

Step 3. Run the SimTool

```
In [6]: r = Run(simToolLocation,inputs)
```

```
submit --local /apps/bin/ionhelperGetArchivedSimToolResult.sh introtosimtools  
r13 RUNS/447c77ed05f446488413f27206d6fcea/inputs.yaml  
RUNS/447c77ed05f446488413f27206d6fcea  
Found cached result
```

introtoolsimtools - workflow notebook

Step 4. Get the outputs

In [7]: `r.getResultSummary()`

Out[7]:

	name	data	encoder	display	filename
0	simToolSaveErrorOccurred	0	text	None	introtoolsimtools.ipynb
1	simToolAllOutputsSaved	1	text	None	introtoolsimtools.ipynb
2	booleanValue	false	text	None	introtoolsimtools.ipynb
3	integerValue	5	text	None	introtoolsimtools.ipynb
4	numberValue	10.7	text	None	introtoolsimtools.ipynb
5	textString	"Now is the time for all good men to come to t..."	text	None	introtoolsimtools.ipynb
6	textFile	file://party.txt	text	None	introtoolsimtools.ipynb
7	imageFile	file://dome_qd_simple.png	text	None	introtoolsimtools.ipynb
8	imageValue	[[[255, 255, 255], [255, 255, 255], [255, 255, ...	text	None	introtoolsimtools.ipynb
9	arrayValue	[[1.0, 2.0, 3.0], [4.0, 5.0, 6.0], [7.0, 8.0, ...	text	None	introtoolsimtools.ipynb
10	arrayFile	file://2Darray.json	text	None	introtoolsimtools.ipynb
11	listValue	["one", "two", "three", "seven"]	text	None	introtoolsimtools.ipynb
12	listFile	file://list.json	text	None	introtoolsimtools.ipynb
13	dictValue	{"one": 2, "three": 3, "two": 2}	text	None	introtoolsimtools.ipynb
14	dictFile	file://dict.json	text	None	introtoolsimtools.ipynb
15	choiceValue	"apple"	text	None	introtoolsimtools.ipynb
16	elementValue	55.845	text	None	introtoolsimtools.ipynb

introto simtools - workflow notebook

```
In [8]: resultBooleanValue = r.read('booleanValue')  
        print(resultBooleanValue)
```

False

```
In [9]: resultIntegerValue = r.read('integerValue')  
        print(resultIntegerValue)
```

5

```
In [10]: resultNumberValue = r.read('numberValue')  
         print(resultNumberValue)
```

10.7