

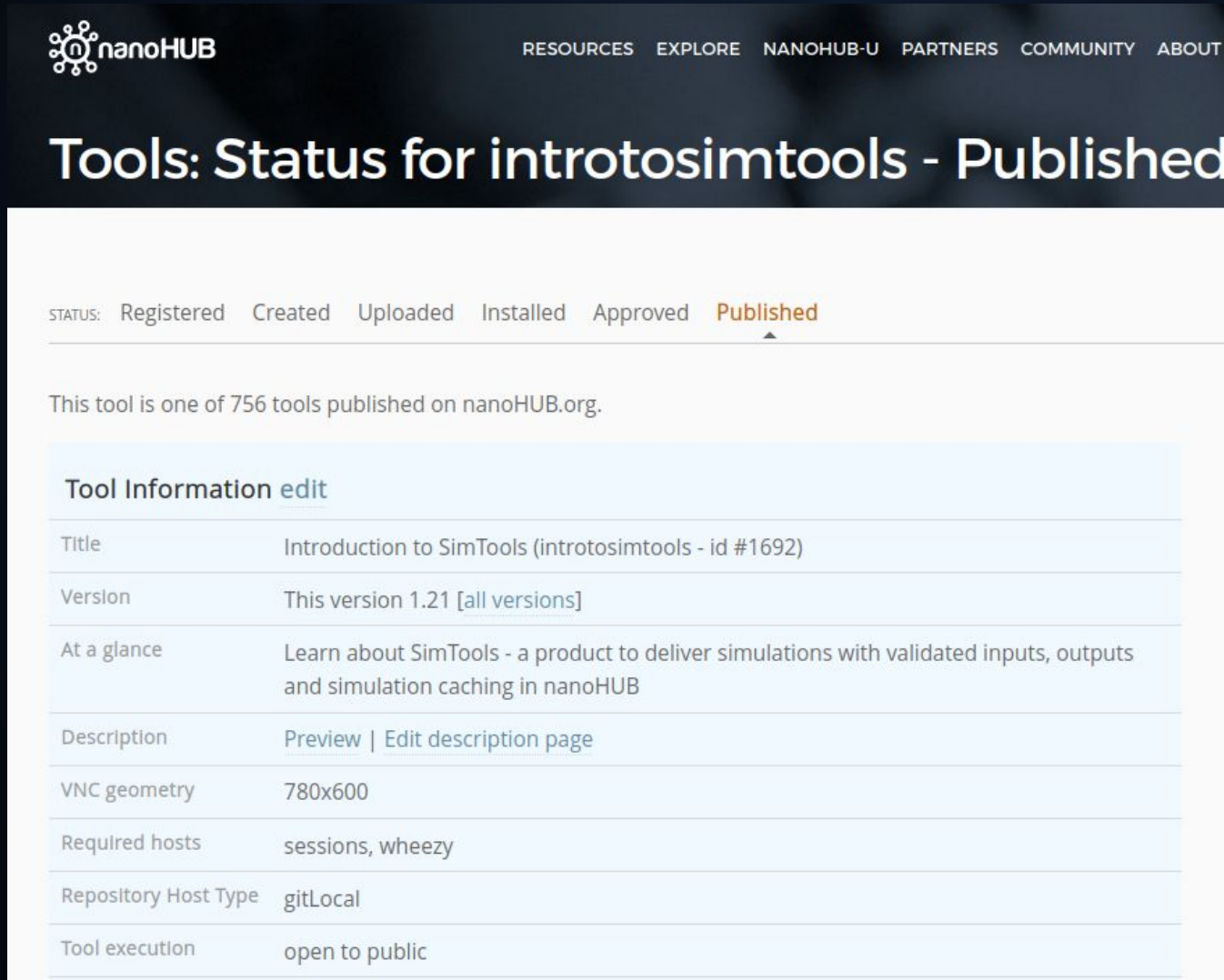
Sim2Ls HUBzero Integration

- Caching
- Access to extended computation resources
 - Singularity containers
 - Anaconda environments
 - HPC
 - GPU

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Sim2Ls HUBzero Integration

- Tool publication achin



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Tools: Status for introtosimtools - Published

STATUS: Registered Created Uploaded Installed Approved **Published**

This tool is one of 756 tools published on nanoHUB.org.

Tool Information edit	
Title	Introduction to SimTools (introtosimtools - id #1692)
Version	This version 1.21 [all versions]
At a glance	Learn about SimTools - a product to deliver simulations with validated inputs, outputs and simulation caching in nanoHUB
Description	Preview Edit description page
VNC geometry	780x600
Required hosts	sessions, wheezy
Repository Host Type	gitLocal
Tool execution	open to public

Sim2Ls HUBzero Integration

- Tool publication
 - DOI
 - Web of Science
 - Google scholar

Introduction to SimTools

By Saaketh Desai, Steven Clark, Alejandro Strachan

Learn about SimTools - a product to deliver simulations with validated inputs, outputs and simulation caching in nanoHUB

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Version 1.01 - published on 04 Oct 2021

doi:10.21981/W91P-6R20 cite this

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04 Oct 2021

Abstract

This tool demonstrates SimTools, the latest way to deliver online simulations in nanoHUB. SimTools are Jupyter notebooks that include declarations of inputs and outputs and a simulation workflow to obtain the outputs from the inputs. The workflow can include physics-based simulations together with pre- and post-processing, or a simple function evaluation. SimTool developers declare inputs (including units and ranges) as well as outputs and the SimTool libraries validates inputs before executing the workflow. SimTool runs that execute correctly and result in valid outputs are automatically added to the nanoHUB simulation cache, so they do not need to be re-executed if the same run is subsequently requested.

nanoHUB users involve the SimTools from graphical user interface apps (see for example: (<https://nanohub.org/tools/qdotjuptest>) or from workflows (see <https://nanohub.org/tools/meltingkim>).

This tool showcases the mechanics of setting up a SimTool and an associated workflow, describing the variety of input and output types possible and the basics of setting up a Run and saving results in the nanoHUB cache. SimTools documentation can be found at: <https://simtool.readthedocs.io/en/latest/>

Cite this work

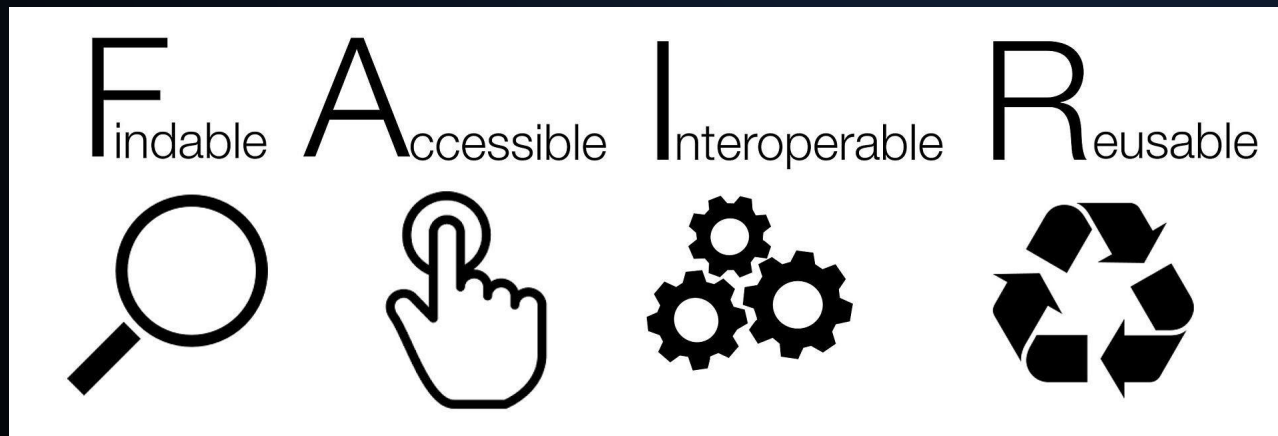
Researchers should cite this work as follows:

Saaketh Desai, Steven Clark, Alejandro Strachan (2021), "Introduction to SimTools," <https://nanohub.org/resources/introtosimtools>. (DOI: 10.21981/W91P-6R20).

[BibTex](#) [EndNote](#)

Summary – Sim2L features

- End to end computational workflow (Repro)
- Published Sim2Ls:
 - Are containerized (Repro)
 - Have DOIs and are indexed by Web of Science & google scholar (F,A)
- Declared and validated inputs and outputs (R, I)
- Services, including metadata, are queryable (F, A, I)
- Automatic result caching (A, R, I)



+ **Repro**ducible

Additional resources

- Sim2L Documentation
 - <https://simtool.readthedocs.io/en/latest/>
- Explore a Sim2L example including all possible IN/OUT types
 - <https://nanohub.org/tools/introsimtools/>
- Learn about nanoHUB software development environment
 - Overview of possible app/tool types & publication process:
 - <https://nanohub.org/whypublish>
 - Working with Jupyter in nanoHUB:
 - <https://nanohub.org/resources/34611>

Questions/Discussion

