



# Software Automation for Research and Training in Neural Engineering

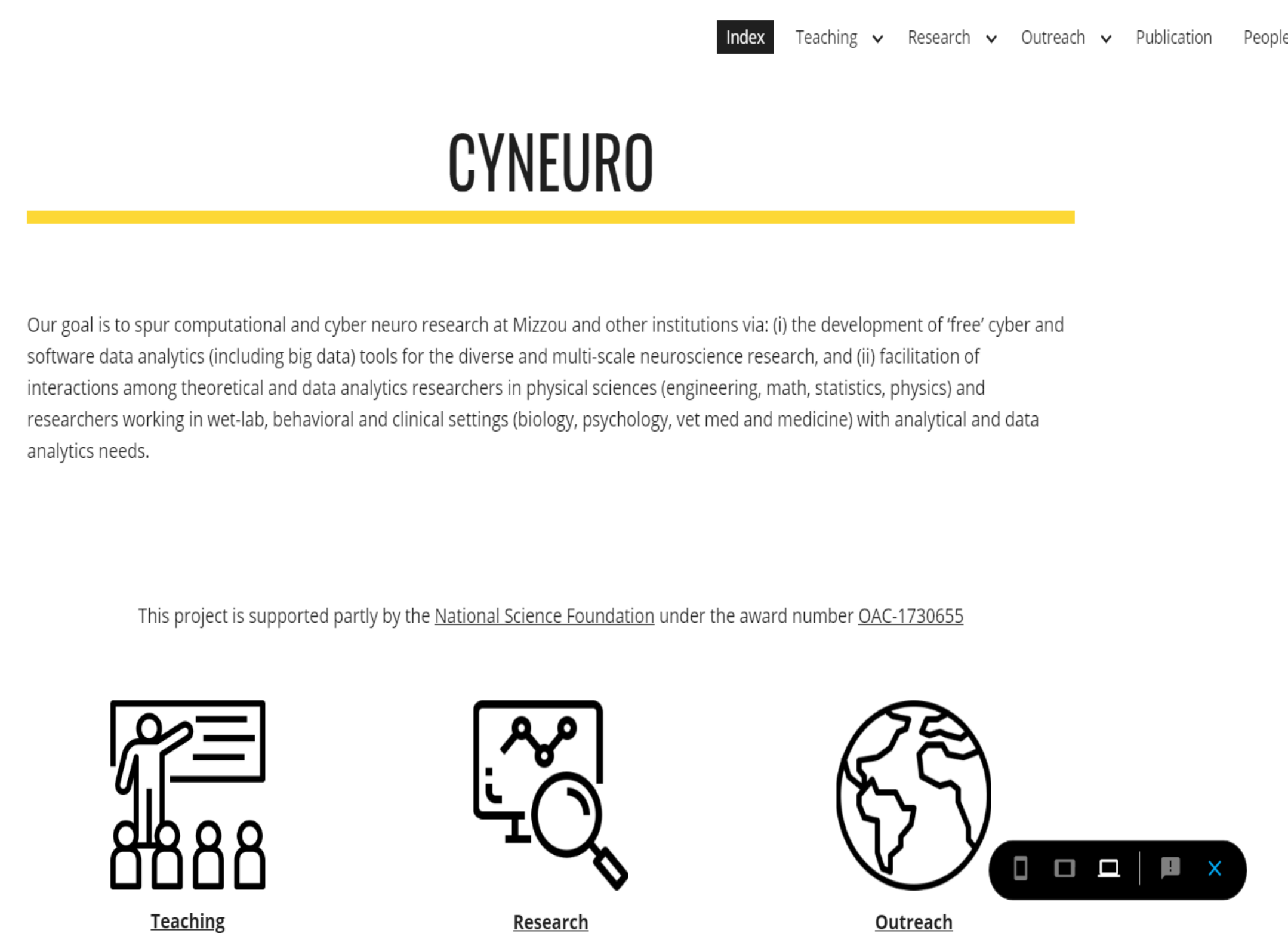
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## Introduction

- Research and training in neuroscience - need for heterogeneous software and data analytic tools, multiple data archives and computing resources.
- Effective use of such resources and technologies is essential for bold advances in neural science and engineering, including bridging across the various ‘levels’ in neuroscience.
- Development of appropriate software automation and cyberinfrastructure (CI) technologies critical to accomplish this without taking valuable time of the neuroscientist from pursuit of knowledge discovery
- We report several automated modules for research and training: transcriptomics (RNAseq) analytic tool; job submission tool SimAgent.

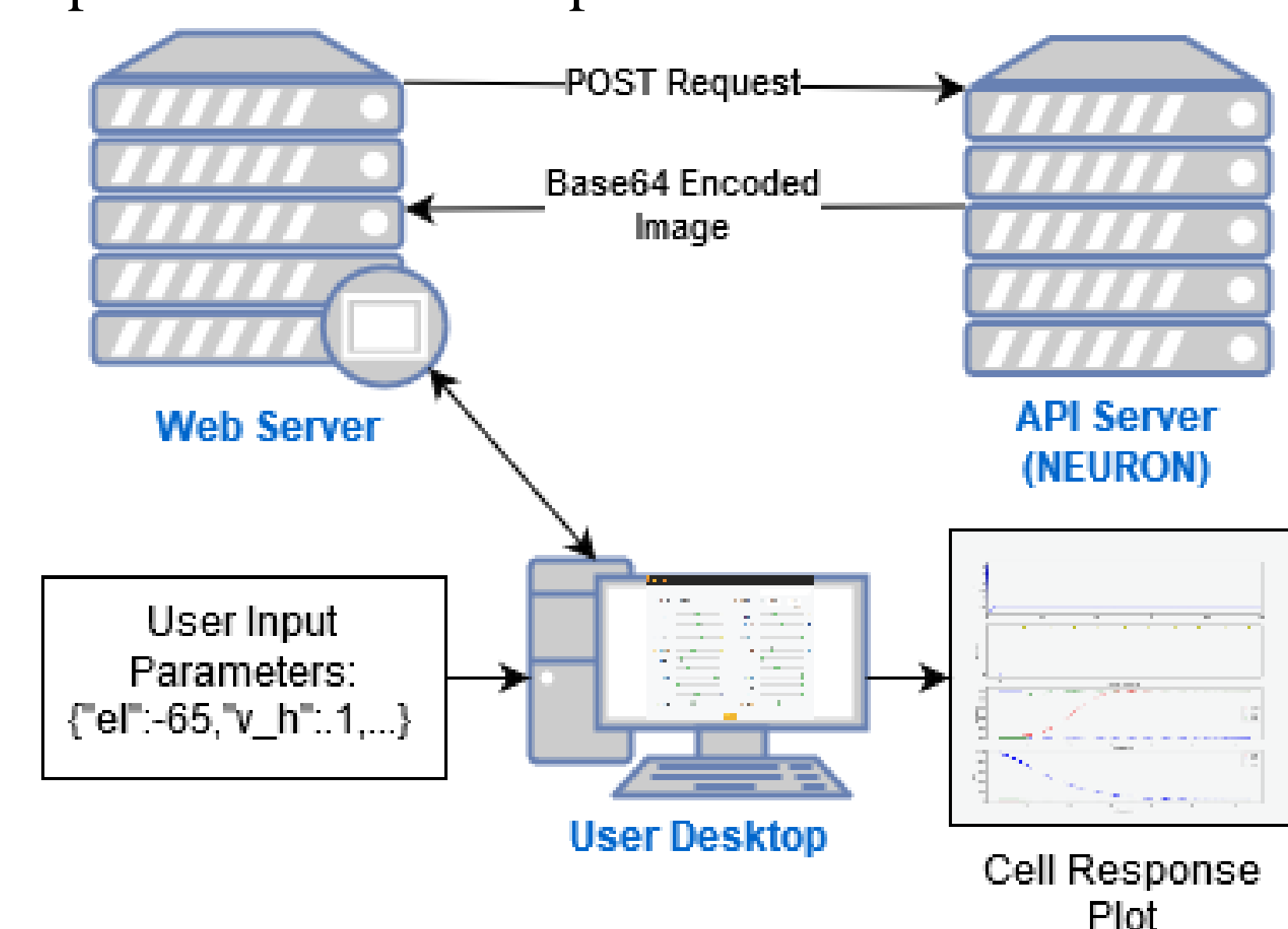
## CyNeuro Portal



**Figure 1:** Public portal to host research and teaching tools above. Also serves as gateway to HPC resources (e.g., XSEDE), and to coordinate summer programs for training and for outreach to K-12

## Automating modules

We have developed different single neuron model development options for teaching and self-learning, using NEURON (1), Jupyter Notebook, and brain machine tool kit (BMTK); 2): (i) using NEURON and GUI; (ii) using Jupyter notebooks with NEURON, BMTK; (iii) with BMTK directly; We have also developed Jupyter notebook modules for cellular neuroscience topics such as Nernst and rest potential, spike generation, bursting, synaptic transmission, and the development of small networks. A JupyterHub server was established on the JetStream cloud computing platform to host several of the notebooks for teaching purposes, an example of which is also provided.



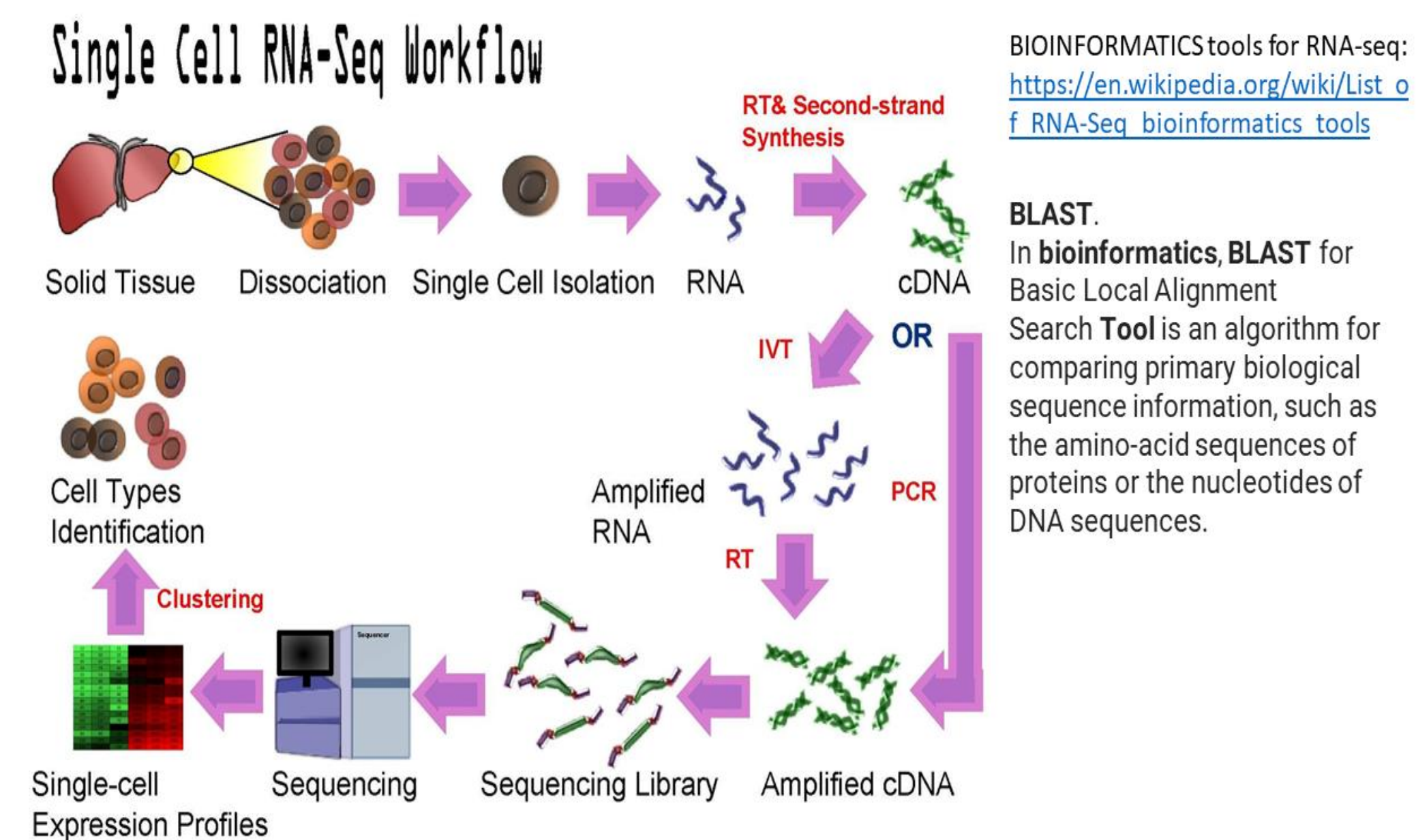
**Figure2:** Automation in tuning 1 component cell

## Single Cell Development Process

- The user enters their desired cell specifications into the webpage
- The parameters are passed from the simple web server to an API server running NEURON
- The API server runs the specified simulation and a returns base64 encoded text containing an image of relevant plots
- The plots are displayed to the user, and the user is given the option to tune the cell further
- Future work includes: multi-compartment cells, large scale networks, teaching tools, and cloud based neuroscience tools with a desktop-like experience

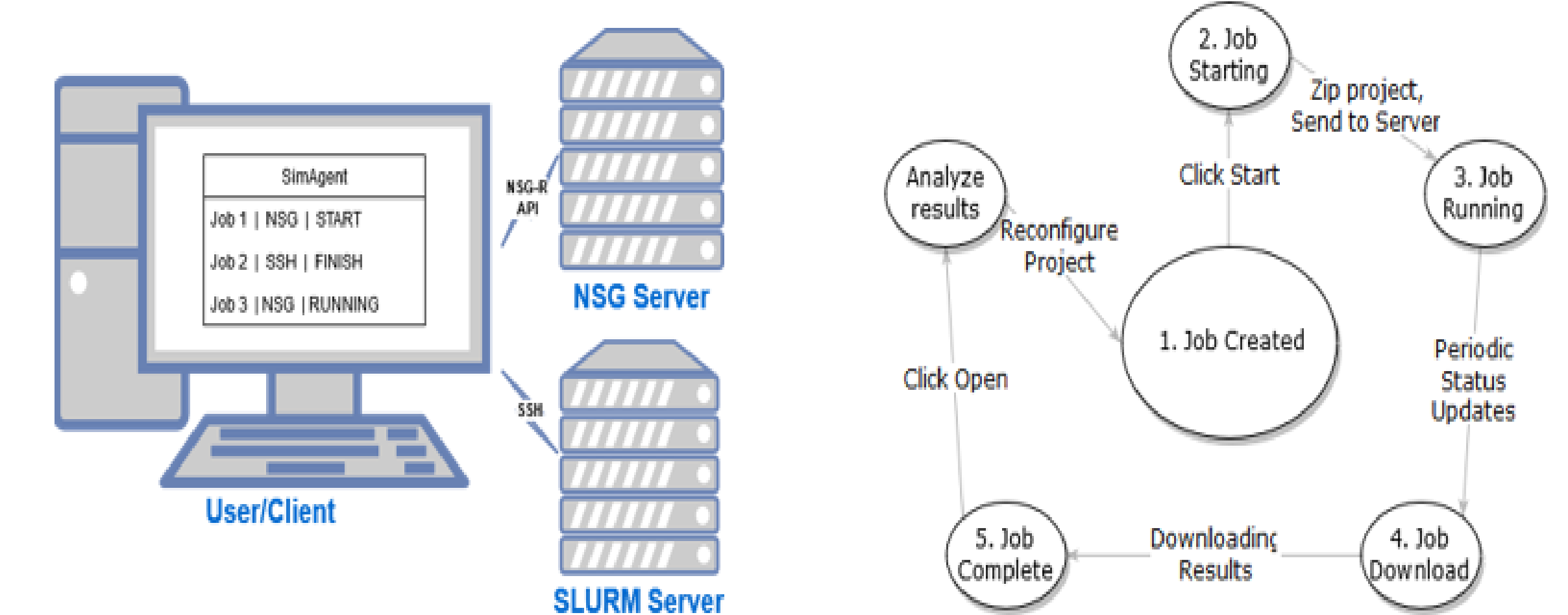


## Transcriptomics Workflow Automation



The identification of differential gene expression between specific conditions is a key in the understanding the phenotypes. The high-throughput transcriptome sequencing (RNA-Seq) has become the main choice to measure gene expression. Consequently, we have developed a protocol to analyze RNA-Seq differential gene expression. The protocol begins with the raw sequencing reads, measures gene expression and lists the significant genes which are differentially expressed between two or more conditions. To efficiently facilitate the workflow, we implement the workflow using the Pegasus workflow management system (Pegasus-WMS) and integrated and optimized the workflow using the Extreme Science and Engineering Discovery Environment (XSEDE) high-performance computing (HPC) virtual system and Cyverse cloud data storage resources.

## SimAgent and NeuroVM virtual machine



**Figure 3.** Representation of a client system connecting to supercomputer (NSG/SLURM) resources using SimAgent (left). Internal SimAgent process for building, configuring, submitting and receiving simulation results (right).

- In addition to the single neuron module described above, we have a software module for automating network models, titled ‘SimAgent’ (Fig.3), that directly interfaced the student laptop with NSG resources to run network simulations.
- **SimAgent** has two core functions, automated job submission and parameter sweep. The automated job submission feature is a point and click interface that accepts any neuron or python program directory, submits the program to run remotely and watches it until completion with live updates to the user. The parameter sweep feature allows the same functionality with the added ability to specify sections of code to automatically change with each run. Users can specify a range of values for a parameter to take on, run each simulation in a parallel configuration and determine the optimal output for their needs. It currently supports connections to the NSG-R restful API and connections using SSH to servers running Slurm. SimAgent can be obtained here: <https://tylerbanks.net/SimAgentMPI/>

**NeuroVM** is a pre-built virtual appliance with all the tools you need to conduct large scale computational neuroscience simulation. This is a resource for individual researchers working on their laptops, and for teaching at introductory college and high school levels. It bundles the following software: Neuron 7.5, Anaconda 3, Nest, BMTK, SimAgentMPI, BMTTools, and VSCode.

NeuroVM can be obtained here: <https://tylerbanks.net/projects/neurovm/>

**CloudNeuro** is a work in progress, and consists of dynamically built Docker images containing neuroscience tools made accessible via remote X11-forwarding capable SSH session. Process:

1. Educators request a registration key from the infrastructure manager through a signup page requesting use case, number of students, type of image to be built (for different tools), etc.
2. The keys issued to the educator will have a use limit (ex: 10) set by the manager and expiration date (ex: Jan 2021) for the remote tools to expire
3. Web page with registration for students will contain standard email password signup with registration key entry, given by their educator
4. Once verified, a Docker image will be built for the student and an address will be given to them for their remote access. MobaXTerm for Windows and Xquartz for Mac preferred.

## Outreach - Summer Courses and K-12

We are developing training materials as well as lesson units that include some of the software automation modules, e.g., Jupyter Notebook implementation of basics related to brain waves.

## References

1. Carnevale and Hines (2006) The NEURON Book;
2. Gartiy et al. (2018) PLOS ONE

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