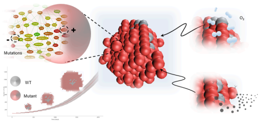
Nov 29, 2018 Version 1

microC: A 3D virtual microenvironment for perturbation biology V.1



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We use this protocol and it's working

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Keywords: signalling networks, gene networks, molecular pathways, genotype to phenotype, agent-based modelling, microenvironment, executable biology, 3d virtual microenvironment for perturbation biology microc, multiscale virtual microenvironment for perturbation biology, perturbation biology microc, 3d virtual microenvironment, multiscale virtual microenvironment, experiment with microc, microc, gene network modelling, surrounding microenvironment, perturbation biology, interactions among cell, easy access to advanced computational modelling, simulation, cell, phenotype, genotype, advanced computational modelling, gene

Abstract

microC is a multiscale virtual microenvironment for perturbation biology. It enables experiments that link genotype to phenotype taking into account the surrounding microenvironment. microC has a modular architecture that enables a wide variety of experiment. Furthermore, it offers easy access to advanced computational modelling and supercomputing resources to the wider scientific community.

microC combines agent-based and gene network modelling and uses partial differential equations to simulate interactions among cells.

The tool itself does not require any installation on the user's machine, as it can be accessed using a web browser. Experimental results and data are also available via a web interface. This protocol describes the process of preparing and submiting an experiment with microC, and interpreting the simulation results

Attachments

PDF

microC-detailed-prot...

1.3MB

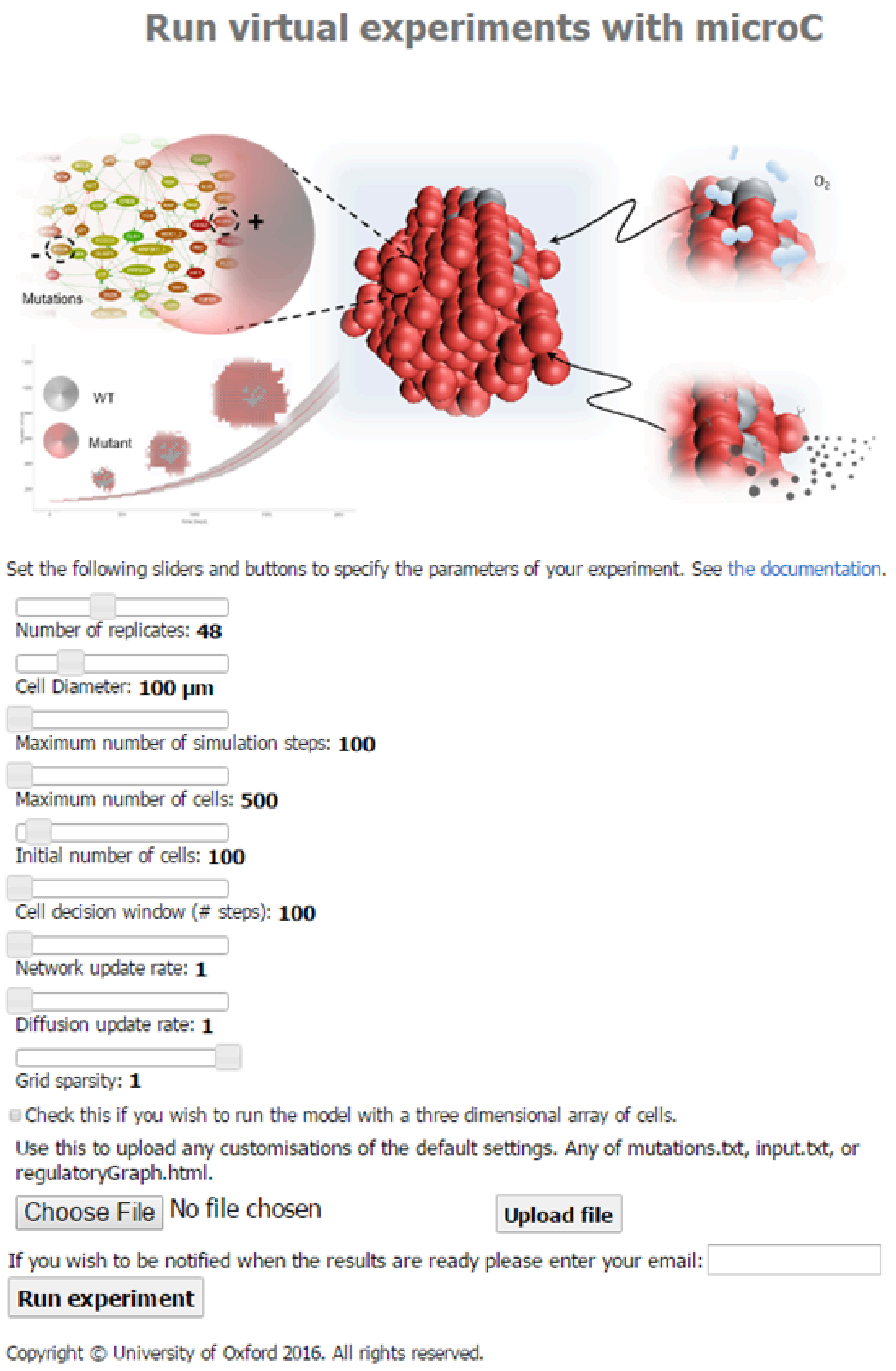
Troubleshooting

Accessing microC

1 microC is available via **microc.org**. During the first visit this step might take several seconds. This will not be the case in future visits.

Preparing an experiment

2 Experiments are specified via the microC main web page (Figure 1). The user may set a number of numerical parameters via sliders, specify the gene network, mutations, and parameters that control diffusion (please, refer to the *microC-detailed-protocol.pdf* for more details). microC modules are enabled through the specification files. For example setting parameters for *Oxygen* or any output node within diffusion-parameters.txt, will automatically enable a diffusion module for this substance. The "Run expreriment" buttom submits the expreriment to the computing cluster.



Run virtual experiments with microC

Set the following sliders and buttons to specify the parameters of your experiment. See the documentation.

Number of replicates: **48**

Cell Diameter: **100 µm**

Maximum number of simulation steps: **100**

Maximum number of cells: **500**

Initial number of cells: **100**

Cell decision window (# steps): **100**

Network update rate: **1**

Diffusion update rate: **1**

Grid sparsity: **1**

☐ Check this if you wish to run the model with a three dimensional array of cells.

Use this to upload any customisations of the default settings. Any of mutations.txt, input.txt, or regulatoryGraph.html.

If you wish to be notified when the results are ready please enter your email:

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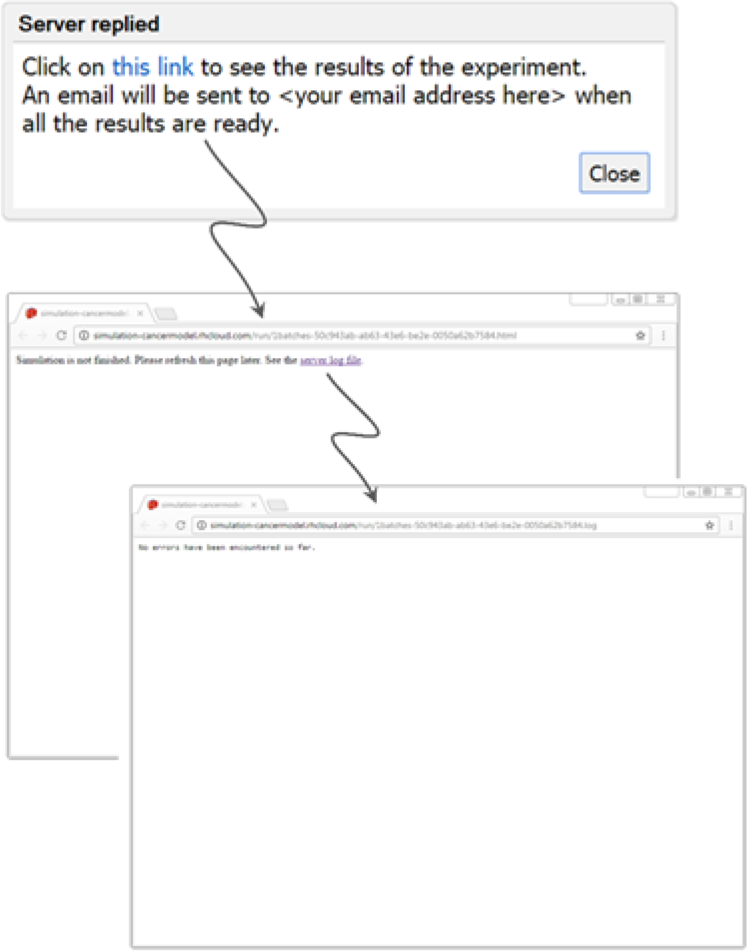
Figure 1. microC main Interface. Sliders are used to setup the numerical parameters, whereas the “Choose File” button may be used to upload local files that define the experiment. The check box enables switching between 2D/3D simulating environment. Finally, the “Run experiment” button submits the experiment.

Submitting an experiment

3 Upon submission of the experiment ("Run Experiment" button, Figure 1) the user receives a link (Figure 2) that provides information about the status of the submission and the log file, where potential errrors are shown. Once the experiment has finished the same link will contain the results (that gradually become available in batches 16 replicates). Optionally, the user will be notified by email.



Server replied

Click on this link to see the results of the experiment.
An email will be sent to <your email address here> when all the results are ready.

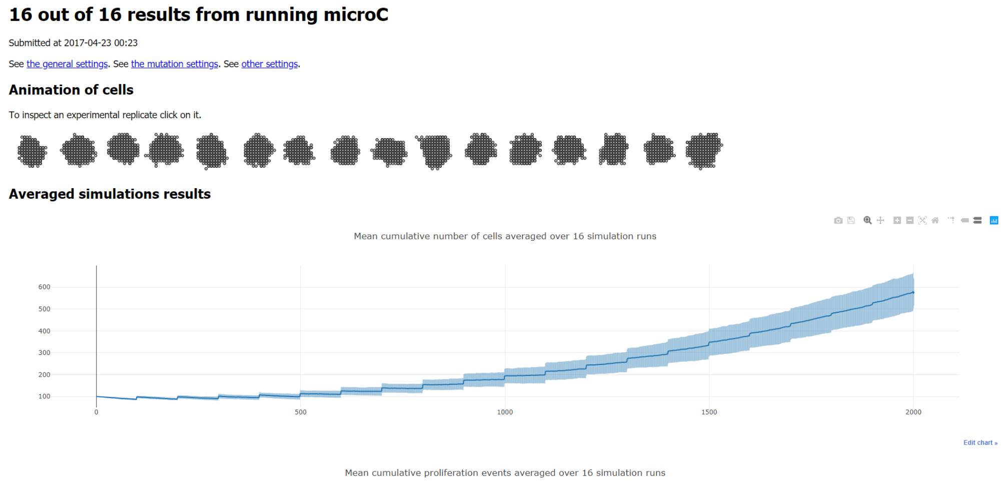
Simulation is not finished. Please refresh this page later. See the server log file.

No errors have been encountered so far.

Figure 2. Upon sumission the user receives a confirmition and a link that will contain the results when the simulations will be finished.

Evaluating the results

4 The results page displays data across all replicates and permits the viewer to inspect any of the replicates in detail. An animation of all replicates is displayed in the initial page along with averaged and detailed data for each of the experimental replicate (Figure 3). A more detailed presentation of the results page is available in the documation page of microc (http://microc.org), or *microC-detailed-protocol.pdf* .



16 out of 16 results from running microC

Submitted at 2017-04-23 00:23

See the general settings. See the mutation settings. See other settings.

Animation of cells

To inspect an experimental replicate click on it.

Averaged simulations results

Figure 3. microC results overview. Results are displayed as animations, along with graphs on cell populations and cell decisions. More detailed information on specific replicates are available on clilcking the specific icon.