StochSS: Stochastic Simulation Service

User Guide and Tutorial

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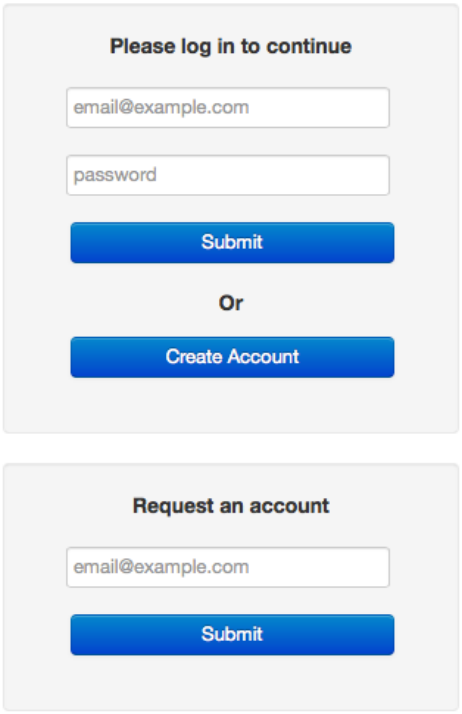
Introduction

1.1 Prerequisites

- StochSS 1.4 (or later) installed on your computer (please follow download and installation instructions at `www.stochss.org`).
- A basic understanding of well-mixed discrete stochastic simulations and models based on ordinary differential equations [1, 2].
- A basic knowledge of the mesoscopic reaction-diffusion master equation and of the Next Subvolume Method (NSM) [7].
- A basic knowledge of the functionalities in the StochSS GUI (please consult the *Basic Introduction to StochSS* tutorial).
- The following login screen appears in your browser; please log in.


Please log in to continue
email@example.com
password
Submit
Or
Create Account
Request an account
email@example.com
Submit

2

Basic Introduction to StochSS

This tutorial will guide you through the basic features of StochSS. You will become familiar with the *Model Editor* and with the *Simulation Manager*. You will learn how to create your own model, which can be *population* or *concentration-based*, and how to simulate it, locally or in the cloud, using either an ordinary differential equation (ODE) solver or the stochastic simulation algorithm (SSA).

2.1 Prerequisites

- The following admin login screen appears upon launch of StochSS:

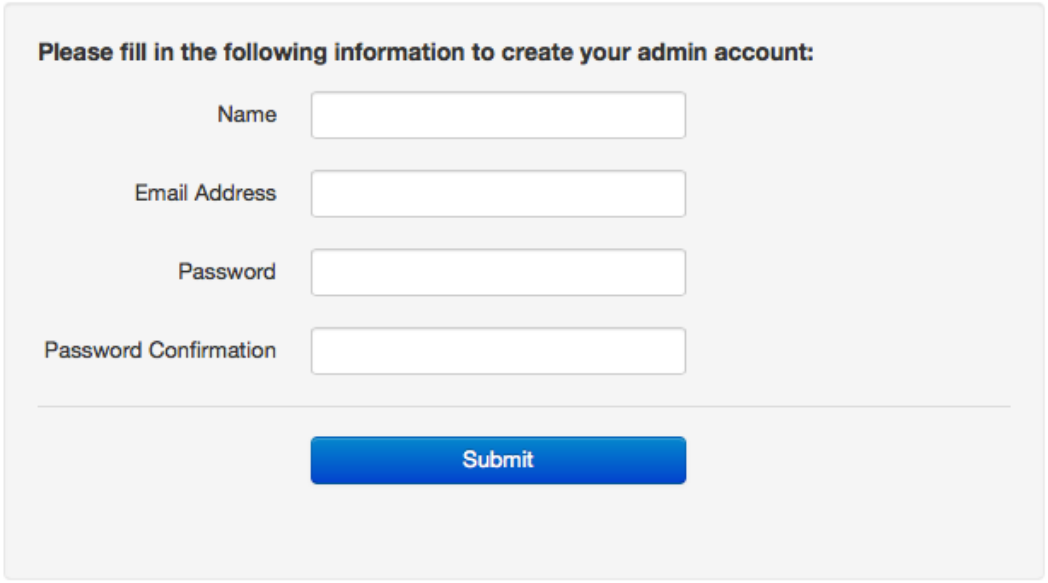


Figure 2.1: Administrator login page

2.2 Creating Administrator and Standard User Accounts

The new user authentication system is currently set up to operate with *one* admin user and any number of regular users. At the end of a successful installation process, your default browser will launch the StochSS server and a the login page will open. You will be asked to create an *admin account*. Once the admin account is created you will be forwarded to a regular login page (Fig. 2.2) where the admin and the approved users can enter the StochSS GUI. The login page also allows users to request an account. The admin user has access to the 'Admin Panel', which has three tables: one for displaying all of the active user accounts in the system ('Active Users' table), one for displaying all of the email addresses of the users who have been approved and haven't created their account yet ('Approved Users' table), and one for displaying all of the email addresses of the users who have requested accounts but have not yet been approved ('Users Awaiting Approval' table). The approved users table allows the admin to delete active users, as well as reset their passwords.

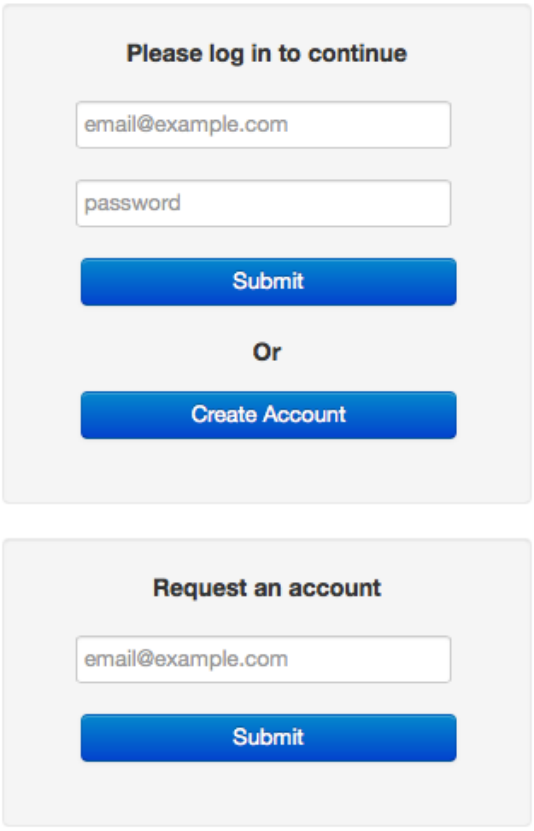


Figure 2.2: User login page

2.3 Importing a Model

The *model editor* will let you create new or modify existing well-mixed stochastic biochemical models as well as deterministic models based on ODEs. The best way to get started with the model editor is to import an example model, and then to browse the different tabs.

Importing an existing StochKit2 model (population model)

Option 1

- **Navigate** to the main Model editor page.
- **Select** the menu *'Import > From File'*.
- **Enter** a model name in the *Name* text box.
- **Select** an XML file. A collection of example models can be found in the directory *examples* within the *StochSS* native folder.
- **Click** on the 'Import' button.

Option 2

- **Navigate** to the main Model editor page.
- **Select** the menu *'Import > Public Library'*.
- **Select** a model from the Public Library **clicking** on Import.
- A pop-up window will appear on your screen allowing you to **name** your model and confirm.

To verify that the model import was successful, navigate back to the Model editor page. At this point we suggest you explore the different tags in the Model editor to become familiar with the StochSS GUI and to take a look at how the different *Species, Parameters* and *Reactions* are defined.

Importing an existing StochKit2 Model (concentration-based model)

StochSS now supports both population and concentration-based models. Concentration-based models are imported the same way as population-based models. It is important to notice at this point that, when the concentration-based model is created and selected, a link to the concentration-to-population conversion page appears on the right side of the screen (Convert to Population).

Converting a concentration model to population

- **Click** on the 'Convert to Population' item on the right to start the conversion process. The model conversion page will open.
- **Click** on the 'Create Model' button at the bottom right of the page to create a population-based model. This newly created population model can be simulated using both deterministic and stochastic solvers.

The conversion process operates correctly only if the model to be converted is entirely based on mass action kinetics. If the model to be converted is NOT entirely based on mass action kinetics, the conversion tool only scales the concentrations to population (integer) values, without modifying the rates (parameters).

2.4 Creating a New Model

As a representative example, we use the dimer-decay population model defined by the following four reactions:

$$\begin{cases} S1 + S1 \underset{\leftarrow c3}{\overset{c2\rightarrow}{\longleftrightarrow}} S2 \xrightarrow{c4} S3 \\ S1 \xrightarrow{c1} \emptyset. \end{cases}$$

The creation of a new model using the Model editor progresses through the following steps:

- **Navigate** to the main Model editor (the 'Model' tag is selected by default).
- **Enter** a model name in the 'Name' text box, **select** the 'Population' button and the 'Non-spatial' button. Finally, **click** on the 'Create model' button.
- **Click** on the 'Species' tag to define chemical species names and their initial values (number of molecules in this case).
- **Use** the 'Add species' button on the right to add *S1*, *S2* and *S3* species with initial populations of $10000, 0, 0$, respectively.
- **Click** on the 'Parameters' tag to define the model parameters' names and their expressions.
- **Use** the 'Add parameter' button to add parameters *c1, c2, c3* and *c4* and their values $1.0, 0.002, 0.5$ and 0.04, respectively.
- **Click** on the 'Reactions' tag to define reaction names, reactants, products and propensities.
- **Use** the 'Add reaction' button to add reactions *R1, R2, R3, R4* (see Fig. 6.6).

2.5 Cloud Computing

You can also use Amazon Elastic Compute Cloud (EC2) to execute your simulation jobs. Using the cloud for your simulation deployments requires that you set up an Amazon Web Services (AWS) account and download your AWS credentials.

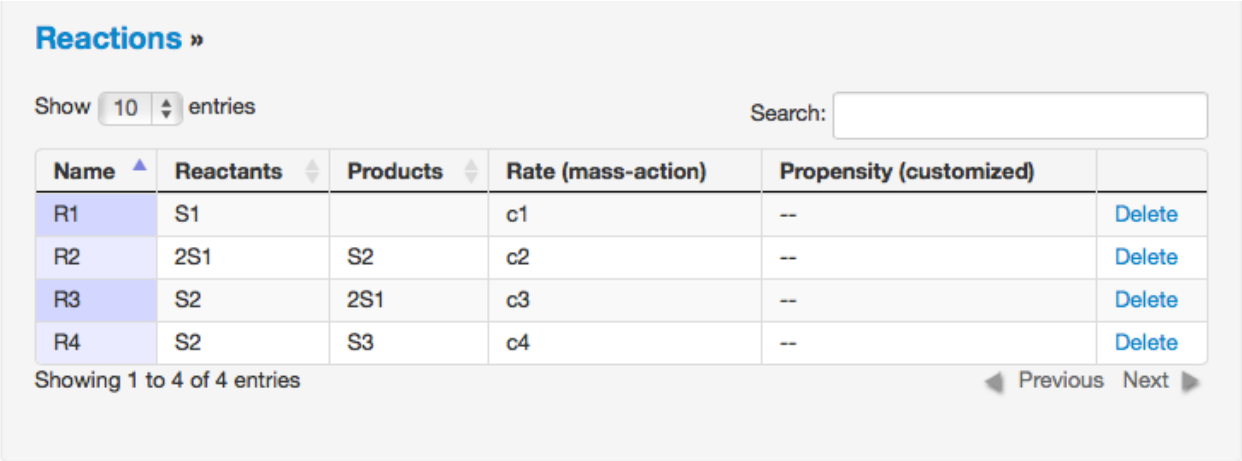


Figure 2.3: Reactions page

Sign up for an Amazon Web Services account (if you do not already have one).

- **Navigate** to `http://aws.amazon.com` and click the 'Sign Up' button.
- An Amazon Web Services (cloud) account requires that you enter credit card information. Amazon will charge for the cloud resources you use via the StochSS app. StochSS automatically shuts down all instances that have been inactive for 2 hours.
- Amazon Micro server instance pricing:
  `http://aws.amazon.com/ec2/pricing/#on-demand`.
- Amazon standard storage pricing (for job results):
  `http://aws.amazon.com/s3/pricing`

Download and save your EC2 credentials

- **Navigate** to *http://aws.amazon.com* and select **Security Credentials** from the 'My Account / Console' menu next to the 'Sign Up' button.
- **Click** the + next to the 'Sign Up' button.
- **Click** 'Create New Root Key'. This process asks you to download and save a file called *rootkey.csv*. Store this file in a safe place. If you lose it, you will have to delete the access key and start again with a new set.
- **Sign out** of the AWS Console by selecting 'Sign Out' from the drop down menu under your name at the top of the page.

2.6 Running a Simulation

Locally

- You can use your local machine (the one on which you deploy and run StochSS) to execute your simulation jobs. [1]
- **Navigate** to the Simulation manager page.
- **Select** the model you wish to simulate and **click** on the 'Next' button. If you are simulating a population-based model you can choose between the deterministic and the stochastic solver. If you choose the deterministic solver, you have the possibility to perform sensitivity analysis on a set of chosen parameters related to your model. Concentration-based models, on the other hand, can only be simulated using the deterministic solver.
- **Setup** your simulation parameters: name, time, data storage frequency, realizations and solver type.
- The default stochastic solver is SSA. To use tau-leaping instead and to define the initial random seed, **click** on 'Advanced Settings'.
- **Click** on the 'Run locally' button. We suggest that you only run small jobs on machines with limited resources.
- **Navigate** to the Job Status page to check the status of your simulation.
- **Click** on the 'View results' link to open the Job summary page where you can plot the simulation's trajectories and download the output files.

In the cloud

Extract your EC2 credentials from the downloaded file.

- Open the *rootkey.csv* file downloaded following the instructions above. You can use a text editor to do so. The file contains two lines:
  AWSAccessKeyId=XXXXXXXXXXXXXXXXXXXXX
  AWSSecretKey=YYYYYYYYYYYYYYYYYYYYYYYYYYYYYYYYYYYY
- **Place** AWSAccessKeyId in the 'Access Key' box on the StochSS Cloud computing page.
- **Place** AWSSecretKeyId in the 'Secret Key' box on the StochSS Cloud computing page.
- **Click** 'Save credentials' when finished.

Launch a Server for StochSS cloud use
Enter ***1*** in the box under 'Compute nodes - Launch new compute nodes' on the StochSS Cloud computing page, and press 'Launch nodes'. After a few minutes, the Status of VMs below this should display 'Running: 1'.

- You can **click** 'Refresh status' to check the status of the VMs.

[1] For Windows users, Amazon EC2 is required. Local execution is not supported at the moment.

- You can **click** 'Stop all nodes' to terminate any running VMs (note that this will also kill any jobs that are running).

Shut down your VMs when you are finished running jobs.

- **Navigate** to the Cloud computing page.
- **Click** on 'Stop all nodes at the bottom of the page.

2.7 Analyzing the Results

- **Navigate** to the Job Status page to check the status of your simulation.
- **Click** on the 'View results' link to open the Job summary page where you can plot the simulation's trajectories and download the output files by **clicking** on 'Access local data'. The simulation's data will be downloaded in your default download folder and will appear either as a zip file or as a new data folder (if you use Safari on a Mac) with a unique name generated from your model's name.

Visualize your data within StochSS
For stochastic simulations you can choose to plot the time series of single realisations or the mean values, and in each of these plots you can simultaneously visualize one or more of your model's species. For deterministic simulations you can plot the time series related to one or more of your model's species together with the corresponding sensitivity analysis data (if this option has been selected).

Access your data for further analysis
For stochastic simulations the data are saved in two subfolders of your data folder named trajectories and stats under the results folder.[c1] For deterministic simulations, the data are saved in a file named output.txt under the results folder.
For cloud jobs, the output folders are not automatically fetched to your local computer. On the Job Status page, you can select a finished job, and then on the page for that job's results, you can choose to fetch the remote data and download it on your local machine. Alternatively, you can obtain all the output data by accessing it in the S3 bucket used by the app. This bucket is available for you to browse from the AWS Console.

2.8 Backup and Transfer your Data

You can backup your saved models from the Backup page which is accessible by clicking on the Backup item in the menu on the left side of your screen.

Create and export a backup archive of your data
From the Backup page, click on the 'Export' button. You will be redirected to the Job Status page. Select the data you want to export/download in the 'Export Job' table at the bottom of the screen. A compressed archive (*zip* file) will be created and downloaded in your default download folder. *Note for Mac users*: Safari automatically decompresses *zip* archives.

[c1] *SH*: I didn't understand this. Is the data saved in subfolders of the folder named 'data', or somewhere else?

Import a backup archive

To create a backup archive from an older version of StochSS execute the following command from a terminal window in the directory of your new StochSS installation:

```
./exportserver.py path_to_your_old_StochSS_installation
```

You can import a backup archive you created with an older version of StochSS. From the Backup page, click on the 'Import' button. You will be redirected to a new page where you can upload a previously created *zip* archive.

3

Sensitivity Analysis with StochSS

3.1 Forward Sensitivity Analysis

StochSS implements forward sensitivity analysis for the deterministic (ODE-based) solver based on the SUNDIAL's CVODES solver [2]. The sensitivity analysis data generated by StochSS are unscaled (and so are the sensitivity analysis plots within the StochSS GUI).

3.2 An Instructive Example

We consider the Michaelis-Menten model that can be imported from the StochSS Public Library (see the *Introduction to StochSS* tutorial for instructions on how to import models in StochSS). Details on the Michaelis-Menten model can be found at the following URL: `http://en.wikipedia.org/wiki/Michaelis-Menten_kinetics`

The snapshot below is from the StochSS simulation page. ***mm*** is the unique name we assigned to the imported Michaelis-Menten model. We perform sensitivity analysis only on the relevant parameters of the model: *mu, k3 Etot, Vmax* and *Km*. On the Reactions page of the ***mm*** model it is easy to see that these are the only parameters that directly affect the values of the species *S* and *P*. Also, note on the same page that the parameter *k3* directly affects only the dynamics of species *P*.

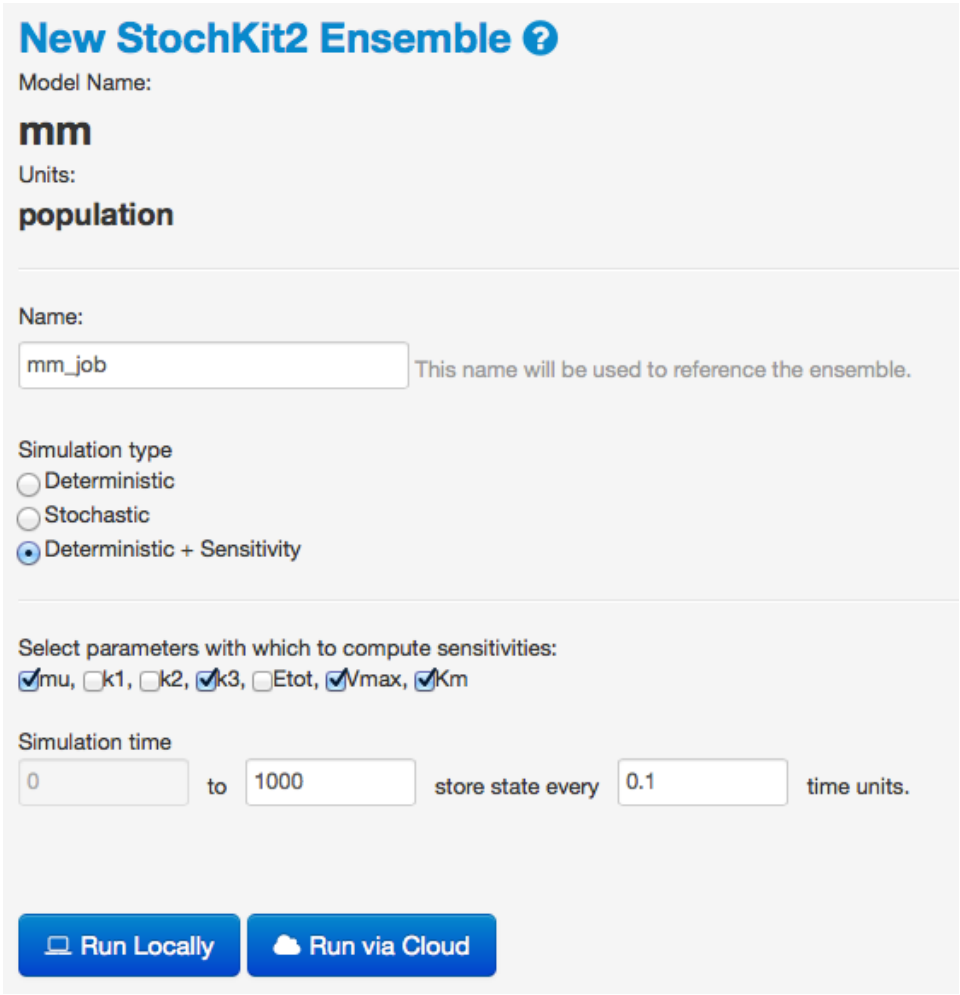
Scaling in sensitivity analysis

Letï£¡s consider the population of *P* and the parameter *Vmax* in our Michaelis-Menten model. The sensitivity of the rate of the increase in population *P* to the parameter *Vmax* is defined as the incremental rate of change in *P* due to incremental changes in *Vmax*:

$$\frac{\partial P(t)}{\partial V_{max}}. \tag{3.1}$$

The analysis of the relative importance of various parameters in determining the dynamic behavior of a population can be negatively affected by the presence of different scales in the parameter set. Hence, for the purpose of comparison, it is preferable to consider scaled **sensitivities** (also called **elasticities**). The elasticity for species *P* with respect to parameter *Vmax* is defined as:

$$\frac{\partial P(t)}{\partial V_{max}} \cdot \frac{V_{max}}{P(t)} = \frac{\partial \log(P(t))}{\partial \log(V_{max})}. \tag{3.2}$$



Using elasticities for parameter comparison is certainly an improvement with respect to the use of unscaled sensitivities. However, it is worth reminding that the use of elasticity may lead to artifacts [3]. After all, elasticity is just one possible transformation that can be applied to the sensitivities. An interesting discussion about sensitivity transformations in ecology is given in Ref. [3].
Among many possible transformation/scaling techniques, we would like to mention the **dimensionless scaled sensitivity** defined as [4]:

$$dss(t, V_{max}) = \frac{\partial P(t)}{\partial V_{max}} \cdot V_{max}, \tag{3.3}$$

and the **composite scaled sensitivity** defined as [4]:

$$css(t, V_{max}) = \sqrt{\frac{\sum_{t=1}^{N} (dss(t, V_{max}))^2}{N}}, \tag{3.4}$$

where N is the number of observations.
Model simulation results will be more sensitive to parameters with larger *elasticities*, *css* and *dss* values.
The following simple *octave*/*matlab* script uploads the data from a simulation run [c0] (file *output.txt*) of the Michaelis-Menten model, implements different scaling procedures and plots some of the results:

[c0] Please consult the *Basic Introduction to StochSS* tutorial for instructions on how to download your simulation data.

```
x = dlmread('output.txt'); % loading the data file
t = x(5:size(x),1); % time array
N = size(t,1); % number of observations
St = x(5:size(x),2); % time series for S
Pt = x(5:size(x),3); % time series for P
% sensitivity analysis for S and P - Km, mu, Vmax, k3
sensiS = x(5:size(x),[4,6,8,10]);
sensiP = x(5:size(x),[5,7,9,11]);
% parameters - Km, mu, Vmax, k3
params = x(3,1:4);
% scaling correction to avoid division by zero
deltaS = 0.0001 * (min(St(St(:, 1) > 0, 1)));
deltaP = 0.0001 * min(Pt(Pt(:, 1) > 0, 1));
% dimensionless scaled sensitivity
%(weight is 1 for all observations)
dssS = sensiS .* params;
elasticityS = dssS ./ (St .+ deltaS);
% composite scaled sensitivity
cssS = sqrt(sum(dssS .* dssS) ./ N);
dssP = sensiP .* params;
elasticityP = dssP ./ (St .+ deltaP);
cssP = sqrt(sum(dssP .* dssP) / N);
figure(1)
plot(t,elasticityS)
title ('Elasticities for S');
xlabel('time');
legend('Km','mu','Vmax','k3','location','northwest');
figure(2)
plot(t,elasticityP)
title ('Elasticities for P');
xlabel('time');
legend('Km','mu','Vmax','k3','location','northeast');
```

4

StochOptim: Parameter Estimation with StochSS

4.1 Prerequisites

- A basic knowledge of the MCEM^2 method [5, 1, 6].

4.2 StochOptim: Parameter Estimation for Stochastic Biochemical Systems

StochSS implements parameter estimation for stochastic biochemical systems (StochOptim) via the Monte Carlo expectation-maximization with Modified Cross-Entropy method (MCEM^2) [5]. MCEM^2 computes maximum likelihood parameter estimates (MLEs) and associated uncertainties in three consecutive phases: cross-entropy, Monte Carlo expectation-maximization (MCEM), and uncertainty quantification [5].

An Instructive Example

We consider the Birth-Death model that can be imported from the StochSS Public Library (see the *Introduction to StochSS* tutorial for instructions on how to import models in StochSS). After the model has been imported:

- **Select** Parameter estimation from the menu on the left of the screen.
- **Click** on the Next button (make sure that the right model is selected). This will open the Simulation page.
- On the Simulation page, **select** only parameter k1. In this example the default value of k2 is already optimized. This is done to make the convergence process faster. Upload the data files that will be used for the parameter estimation.
- Example files (StochOptim input data) for the initial conditions and the trajectories are provided in the *examples* folder (included in your StochSS package) and are named *birthDeathInitial.txt* and *birthDeathTrajectories.txt*, respectively.
- Now we are ready to start the parameter estimation routine clicking on the Run Locally button at the bottom of the page.
- **Select** Job Status from the menu on the left of the screen to monitor the status of your running calculation. **Click** on View Progress to access the Job Summary page and view more details about your

calculation status. *Note:* parameter estimation calculations using MCEM^2 are typically time consuming, intensive calculations. For this simple example, the parameter estimation process took about 9 – 10 minutes on a Macbook Pro (Intel Core i7 - 2011). By selecting both k1 and k2 parameters the parameter estimation process took about 90 minutes on the same machine.

- When the job has successfully ended, you can generate a new model using the final estimates of the MCEM^2 calculation as follows: scroll to the bottom of the Job Summary page and **click** on the Create Model from Current Estimates button.
- If the job doesn't complete in a reasonable amount of time the job can be stopped manually on the Job Status page and the parameters can be extracted using the Create Model from Current Estimates button.

StochOptim file format

The StochOptim input data format consists of two, tab-separated text-based input files. The first file represents the initial conditions of the system, and the second file represents trajectories of it. Each file has three base columns. *Time*, *Rep*, and *Weight*. Additional columns are added for every species in the model that parameter estimation is to be run on. The *Time* column contains the time values of the various trajectories (and should be set to zero for the initial conditions file). The *Rep* column is used to include multiple trajectories in one file for fitting. Basically each trajectory should have a different *Rep* number. An example of this can be seen by comparing the files *birthDeathTrajectories.txt* and *birthDeathTrajectoriesMulti.txt* in the *examples* folder included in the StochSS package. The *Weight* column is currently unused and should be set to 1. The rest of the columns should be named after the species (case-sensitive) in the model the data will be fit against, and the columns themselves should contain integers representing the population counts at the various time points.

5

Spatial Stochastic Simulations with StochSS

5.1 Prerequisites

- A basic knowledge of the mesoscopic reaction-diffusion master equation and of the Next Subvolume Method (NSM) [7].

5.2 Spatial Stochastic Simulations

The spatial stochastic simulation capabilities in StochSS are based on PyURDME [8]. PyURDME is a general software framework for modeling and simulation of stochastic reaction-diffusion processes on unstructured, tetrahedral (3D) and triangular (2D) meshes. Unstructured meshes allow for a more flexible handling of complex geometries compared to structured, Cartesian meshes. The current core simulation algorithm is based on the mesoscopic reaction-diffusion master equation (RDME) model. The default solver is an efficient implementation of the NSM.

An Instructive Example

We will build a simple model based on an annihilation reaction between two chemical species generated by sources located at the two opposite bases of an enclosing cylinder.

The creation of our new spatial model using the Model editor progresses through the following steps:

- **Navigate** to the main Model editor (the 'Model' tag is selected by default).
- **Enter** a model name in the 'Name' text box, select the 'Population' button and the 'Spatial' button. Finally, **click** on the 'Create model' button.
- **Click** on the 'Species' tag to define chemical species names and their diffusion coefficient.
- **Use** the 'Add species' button on the right to add A and B species both with diffusion coefficient $D = 1$.
- **Click** on the 'Parameters' tag to define model parameters names and their expressions.
- **Use** the 'Add parameter' button to add parameter *k1* with a value of 100.
- **Click** on the 'Reactions' tag to define reaction names, reactants, products and propensities.
- **Use** the 'Add reaction' button to add reactions *R1, R2, R3* (see Fig. 6.6). To insert reaction R1 and R2 ('birth' reactions) leave the 'Reactants' text box empty and type in the name of the generated species in the 'Products' text box. To define R3 (the annihilation reaction), enter the species names separated by a comma in the 'Reactants' text box. Leave the 'Products' text box empty. Check out the on-screen help buttons.
- **Click** on the 'Mesh' tag and select 'Cylinder'. You will notice that the cylindrical mesh is divided in three subdomains. Select the proper 'buttons' in sections 3 and 4 on the 'Mesh' page. Keep in mind that species A is generated in subdomain 1, whereas species B is generated in subdomain 3. Both species are allowed to diffuse everywhere within the cylinder (in all three subdomains). In other words, reaction R1 should be limited to subdomain 1 and reaction R2 to subdomain 3. Reaction R3 can happen in all three subdomains.
- **Click** on the 'Add Initial Condition' button and 'Select' 'Scatter', 'A', 'Subdomain = 1','Count = 500'. **Click** ', 'B', 'Subdomain = 3','Count = 500'. **Click** on the 'Add Initial Condition' button.
- Your spatial model is completely defined and ready to be simulated.
- **Navigate** to the Simulation manager page.
- **Select** the spatial model you just created and **click** on the 'Next' button.

- **Setup** your simulation parameters: name, time, data storage frequency and realizations.
- To define the initial random seed, **click** on 'Advanced Settings'.
- **Click** on the 'Run locally' button.
- In a few seconds you will be directed to the Job Status page where you can check the status of your simulation.
- Once your simulation is complete, **click** on the 'View results' link to open the Job summary page where you can visualize the diffusion of the two species (A and B) over time within the cylindrical container and download the output files of the simulation.

Figure 5.1: 'Reactions' page

6

Cloud Computing with StochSS

6.1 Credentials

StochSS provides the options to run different types of jobs using the cloud infrastructures. In StochSS 1.2-1.5, the cloud services it has are all by Amazon Web Service (AWS). In order to use AWS Elastic Computing Cloud (EC2), Simple Storage Service (S3) and DynamoDB database, which are all required by running jobs in the cloud, you should be prepared to have at least one AWS account and one credential (access key pair) in hand.

More information regarding how to create an AWS account or a security credential can be found here: `http://aws.amazon.com`

An Instructive Example on Setting Credentials

The StochSS will validate the credentials (access key pairs) you have to be authorized to run job in the cloud.

An example will be shown to you on how to validate your credentials in StochSS through the following steps:

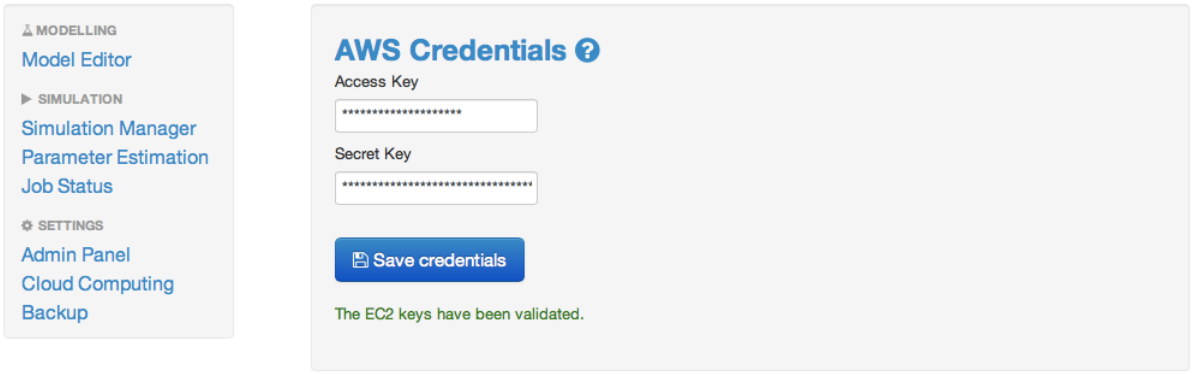


Figure 6.1: 'Cloud Computing' page - 'Credentials' section

- **Navigate** to the main Cloud Computing page by **clicking** the "Cloud Computing' on the side bar.
- **Type in** or **copy** the access key id of your credentials in 'Access Key' text box.
- **Type in** or **copy** the secret access key of your credentials in 'Secret Key' text box.
- **Click** on the 'Save credentials' button to save your credentials into the database. Whenever there is no computing node running (the nodes can be seen in the 'Status of VMs' section down the same page) with your current credentials, you could always change your credentials to another and save to restore them.
- **Double check** the credentials are valid by seeing the message below.

6.2 Compute Node

There are as many as six different types of AWS EC2 compute nodes for you to run your jobs in the cloud: t1.micro, m1.small, m3.medium, m3.large, c3.large, c3.xlarge. These nodes comprise varying combinations of CPU, memory, storage, and networking capacity. Please follow the link to know more about different types of nodes: `http://aws.amazon.com/ec2/instance-types/`.

More information regarding how to create an AWS account or a security credential can be found here: `http://aws.amazon.com`

An Example on Launching and Shutting Down Nodes

Computing node section provides the options of both launching a default node and manually choosing combinations of different nodes at a time. In addition, the status of each launching node can be checked by refreshing the page. Moreover, there is only one click to terminate all running/pending/creating nodes.

An example will be shown on how to launch and shut down nodes as well as refresh the status:

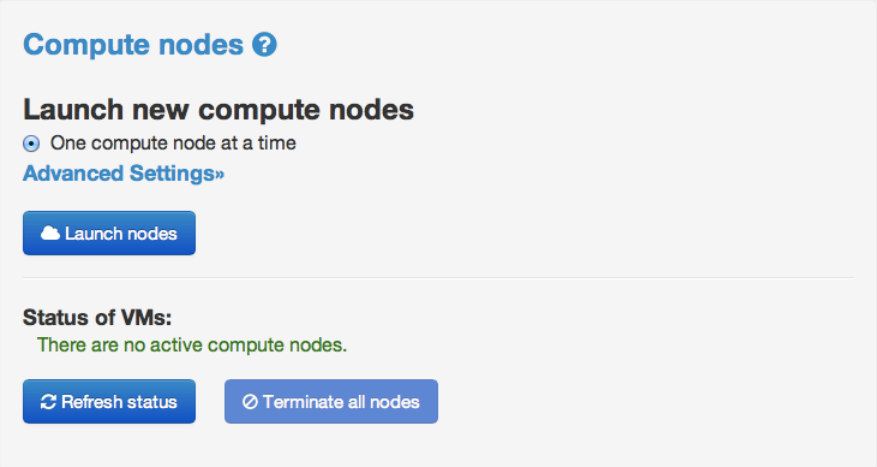


Figure 6.2: 'Cloud Computing' page - 'Compute nodes' default setting section

- **Navigate** to the main Cloud Computing page by **clicking** the 'Cloud Computing' on the side bar. Compute nodes section is right below the Credentials
- 'One compute node at a time' is chosen by default, which means that you could **Click** 'Launch nodes' button directly and that will launch one c3.large node for you for the first time (as a head node) and all t1.micro nodes for the rest.
- By **clicking** the 'Refresh status' button, you are able to check the status of the launching nodes.
- By **clicking** the 'Terminate all nodes' button, you are able to terminate all nodes of all status.

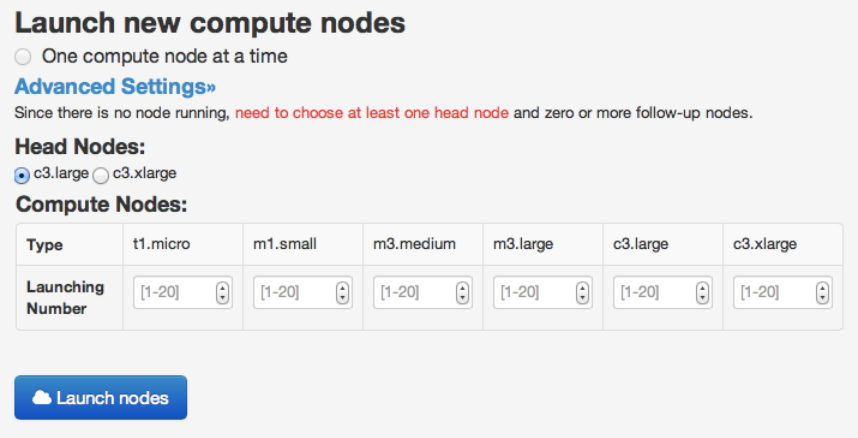


Figure 6.3: 'Cloud Computing' page - 'Compute nodes' advanced setting section

- If you need more options on node types, 'Advanced Settings' will be the right place to take things under control.
- **Choose** one of the 'c3.large' or 'c3.xlarge' if there is no head node running.
- **Input in** more numbers in the text box under the proper types
- **Click** the 'Launch nodes' button to launch the nodes you have chosen previously.

6.3 Reproduction

To repeatedly access the output of a cloud job, StochSS provides the flexibility to both store the output in the cloud or reproduce the job every time it's needed (in order for less storage cost). By figuring out which way is the most economic for both time and money cost, you are encouraged to choose the better way of accessing the output.

An Example on Job Reproduction

An example shown below will guide you on how to reproduce a existing job.

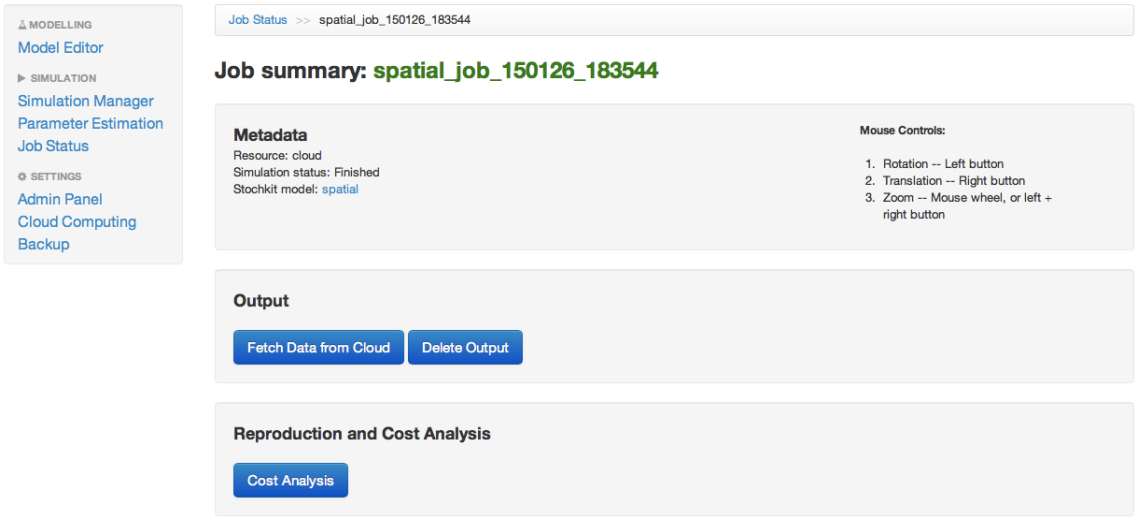


Figure 6.4: 'Job summary' page - 'reproduction' not available

- **Navigate** to Job Status page, which can be found by **clicking** 'Job Status' on the side bar.
- **Click** the 'view' link of the job you would like to reproduce to go to the Job summary page.
- If cloud output is already there to be viewed (show as **FIG 4**), you can either **click** the 'Fetch Data From Cloud' button to view the statistics plot or **click** 'Delete Optput' to delete output in the cloud. Notice that **if there is output already stored in the cloud, no reproduction action is available until you delete the output**.
- If cloud output is not there, thus Output section being blank, the option to reproduce the job will be displayed (shown as **FIG 5**).
- **Choose** the right node type for reproduction. If there is no such type running, a warning will show up to guide you to the Cloud Computing page to launch one.

- **Click** the 'Reproduce Results' button to submit the request. Then it will redirect to the Job Status page for job progress viewing.

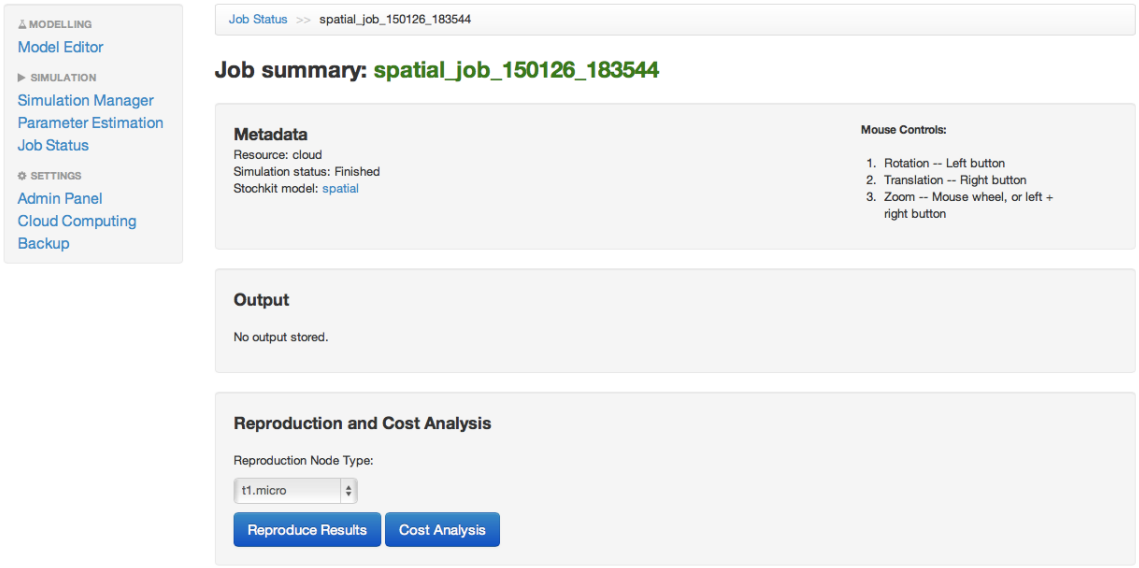


Figure 6.5: 'Job summary' page - 'reproduction' available

6.4 Cost Analysis

To choose the right node type for job reproduction later, StochSS provides the possibility to analyze the time and money cost to run with different types of nodes. The results are plot for more intuitive comparison and best selection.

An Example on Job Reproduction

An example shown below will guide you on how to analyze the cost of reproduce an existing job.

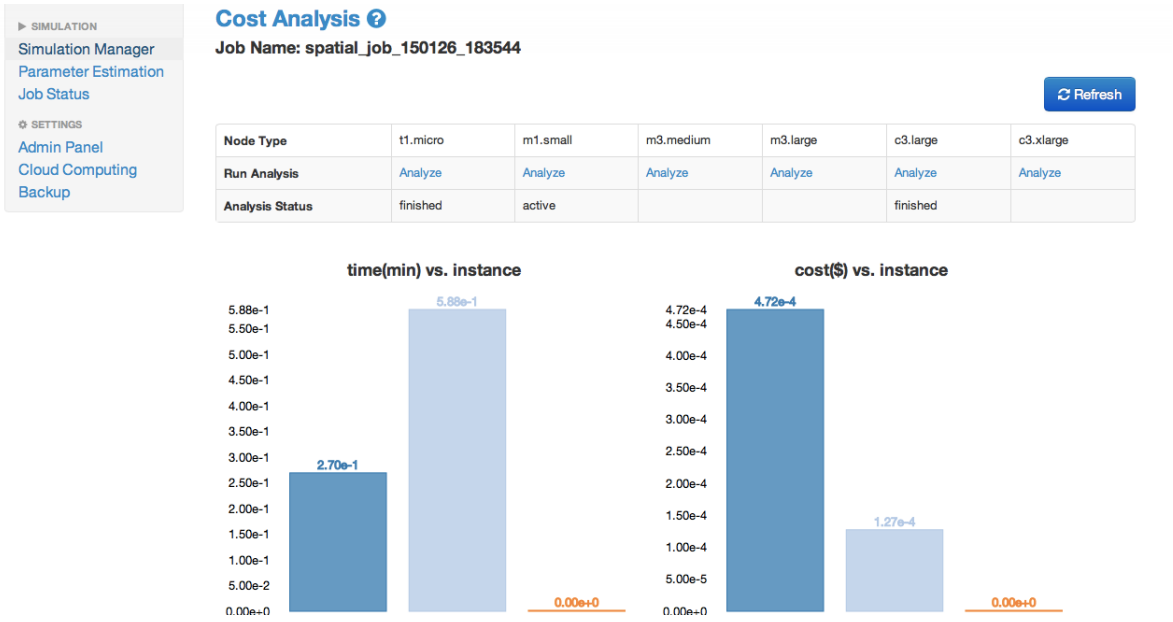


Figure 6.6: 'Cost Analysis' page

- **Navigate** to Job Status page, which can be found by **clicking** 'Job Status' on the side bar.
- **Click** the 'view' link of the job you would like to reproduce to go to the Job summary page.
- **Click** the 'Cost Analysis' button in the Reproduction and Cost Analysis section.
- **Click** the 'Analyze' button with the node type you would like to run and analyze. The page will auto refresh after the request is submitted and show its status of the analysis. If the analysis remaining to be 'active', **click** the 'Refresh' button to refresh the status.
- If the running is 'finished', the time and money cost of running the job with the node type you chose will be plotted in the graph below for comparison.

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[c1] *SH*: 230'6? — check this.