

# StochSS: Stochastic Simulation Service

## An Integrated Development Environment for Simulation and Analysis of Discrete Stochastic Biochemical Models



National Institutes of Health

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### Abstract

We present StochSS: Stochastic Simulation as-a-Service, an integrated development environment for modeling and simulation of discrete stochastic biochemical systems. An easy to use WebUI enables researchers to quickly develop and simulate biological models on a desktop or laptop, which can then be expanded or combined to incorporate increasing levels of complexity. As the demand for computational power increases, StochSS is able to seamlessly scale by deploying cloud computing resources. The cloud computing facilities also makes it possible to deploy StochSS as a multi-user software as-a-service (SaaS) environment with the possibility to share and exchange models via a public model repository. StochSS currently supports simulation of ordinary differential equations and well-mixed discrete stochastic models, as well as parameter estimation of discrete stochastic models and simulation of spatial stochastic models. StochSS is available for download at:

[www.StochSS.org](http://www.StochSS.org)

Try StochSS without downloading at:

[try.StochSS.org](http://try.StochSS.org)



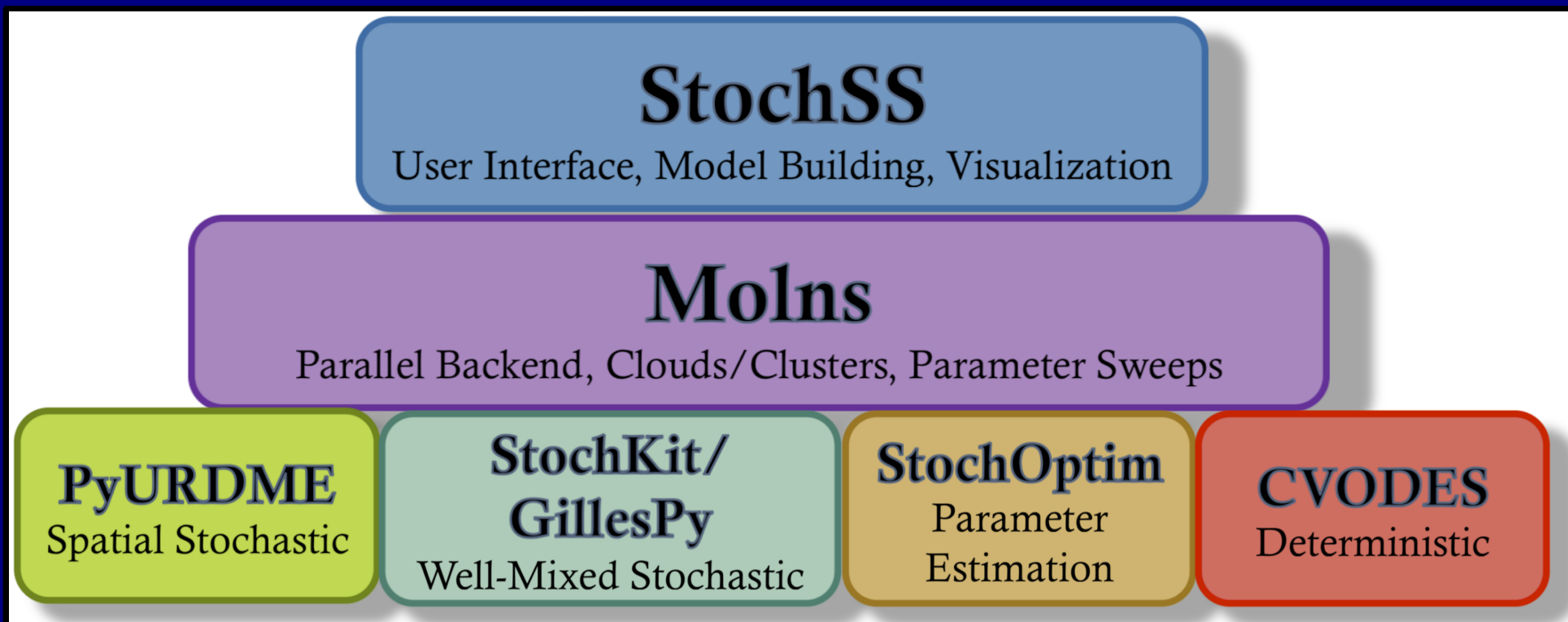
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RESEARCH ARTICLE  
Stochastic Simulation Service: Bridging the Gap between the Computational Expert and the Biologist

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A wide range of powerful computational tools, all in one place!



### CVODE - ODE simulation

CVODES is a solver for stiff and nonstiff ordinary differential equation (ODE) systems with sensitivity analysis capabilities. <http://computation.llnl.gov/casc/sundials/>

### StochKit - Stochastic Simulation

StochKit is an efficient, extensible stochastic simulation framework developed in the C++ language that aims to make stochastic simulation accessible to practicing biologists and chemists, while remaining open to extension via new stochastic and multiscale algorithms. The current version of StochKit includes the popular Gillespie Stochastic Simulation Algorithm (SSA) Direct Method, our new Logarithmic Direct Method which is considerably faster than the original Direct Method, slow-scale SSA for multiscale problems, adaptive non-negativity preserving explicit tau-leaping, and core modules for explicit, implicit and trapezoidal tau-leaping methods. K.R. Sanft et al. *Bioinformatics* (2011)

### StochOptim - Parameter Estimation

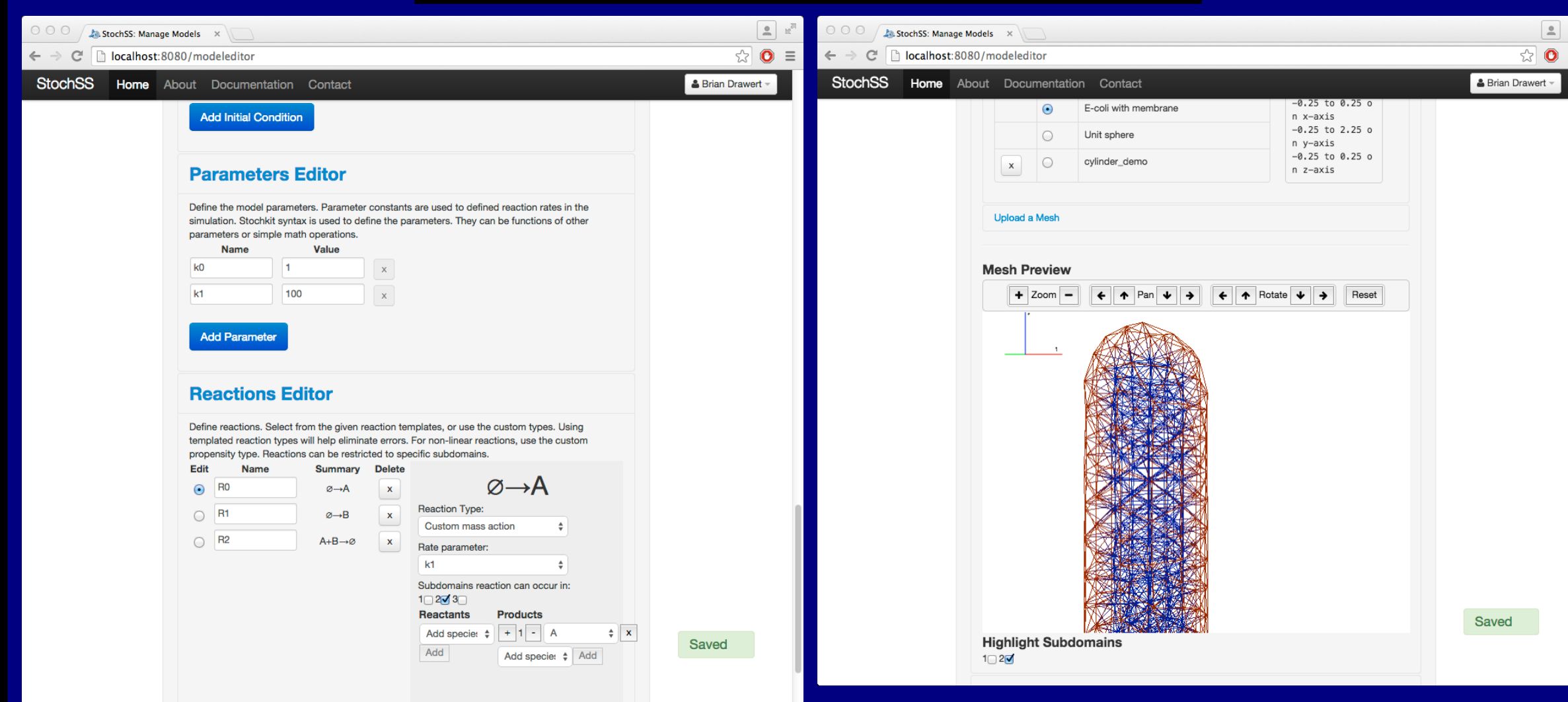
StochSS implements parameter estimation for stochastic biochemical systems (StochOptim) via the Monte Carlo expectation-maximization with Modified Cross-Entropy method (MCEM<sup>2</sup>). MCEM<sup>2</sup> computes maximum likelihood parameter estimates (MLEs) and associated uncertainties in three consecutive phases: cross-entropy, Monte Carlo expectation-maximization (MCEM), and uncertainty quantification. B.J. Daigle et al. *BMC Bioinformatics* (2012)

### PyURDME - Spatial Stochastic

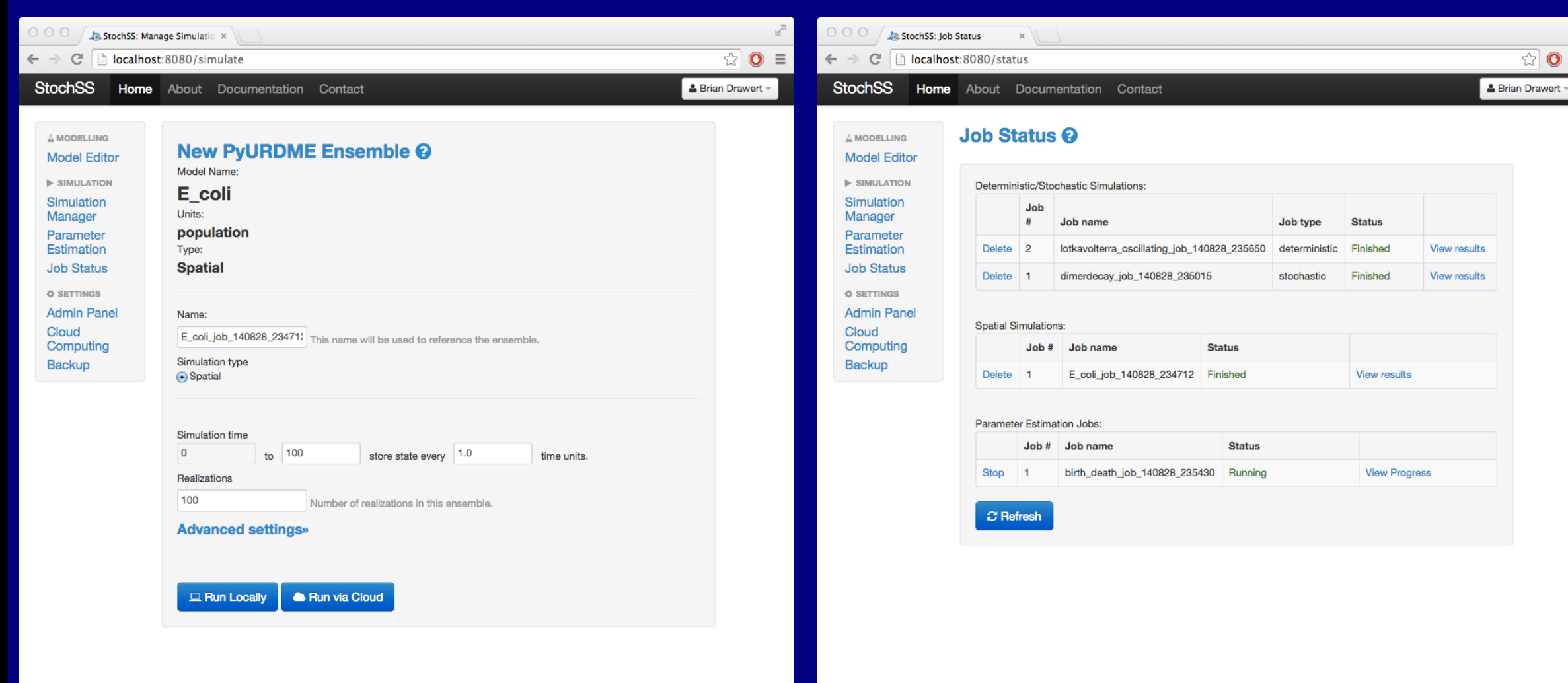
PyURDME is a general software framework for modeling and simulation of stochastic reaction-diffusion processes on unstructured, tetrahedral (3D) and triangular (2D) meshes. The core simulation routines are implemented in C, and requires GCC for compilation. The default solver is an efficient implementation of the Next Subvolume Method (NSM). B. Drawert et al. *SISC* (2016)

### StochSS Workflow

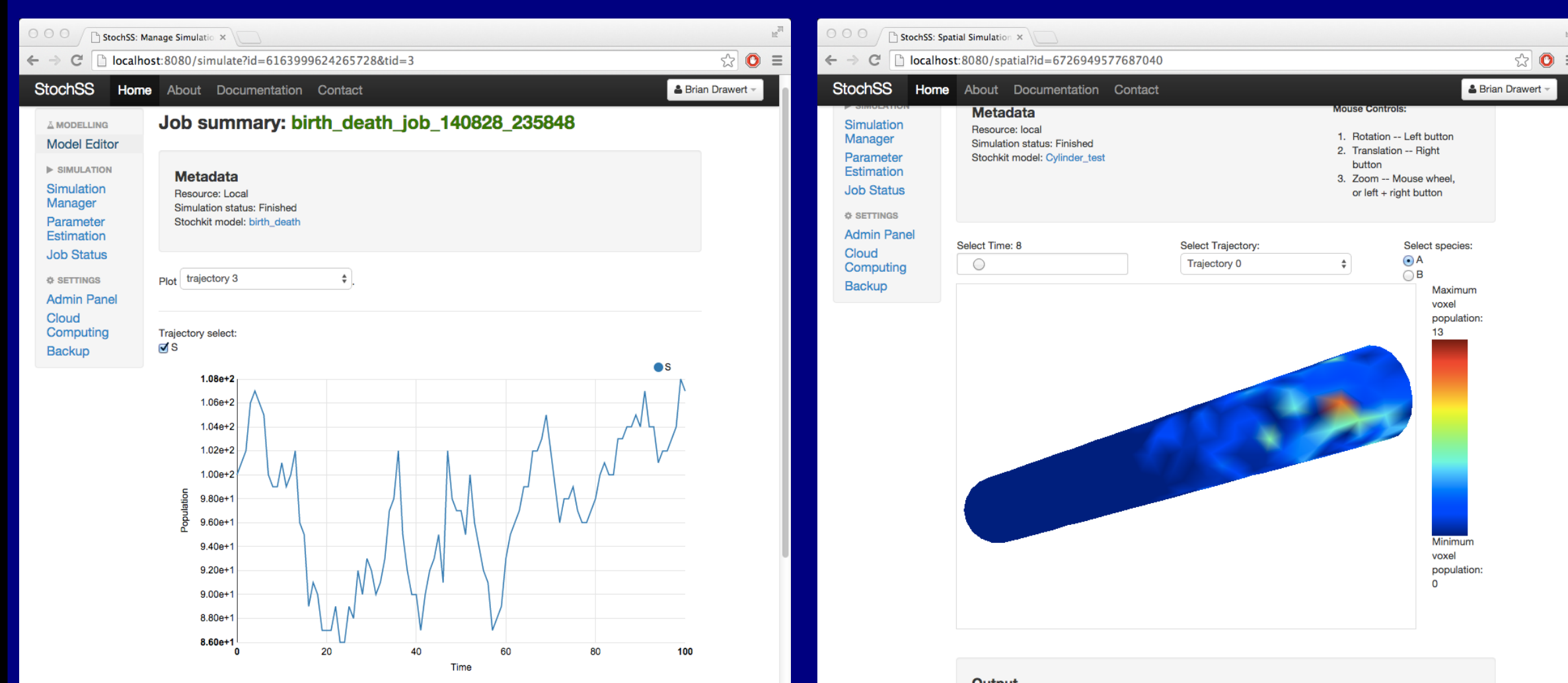
#### Build a Model



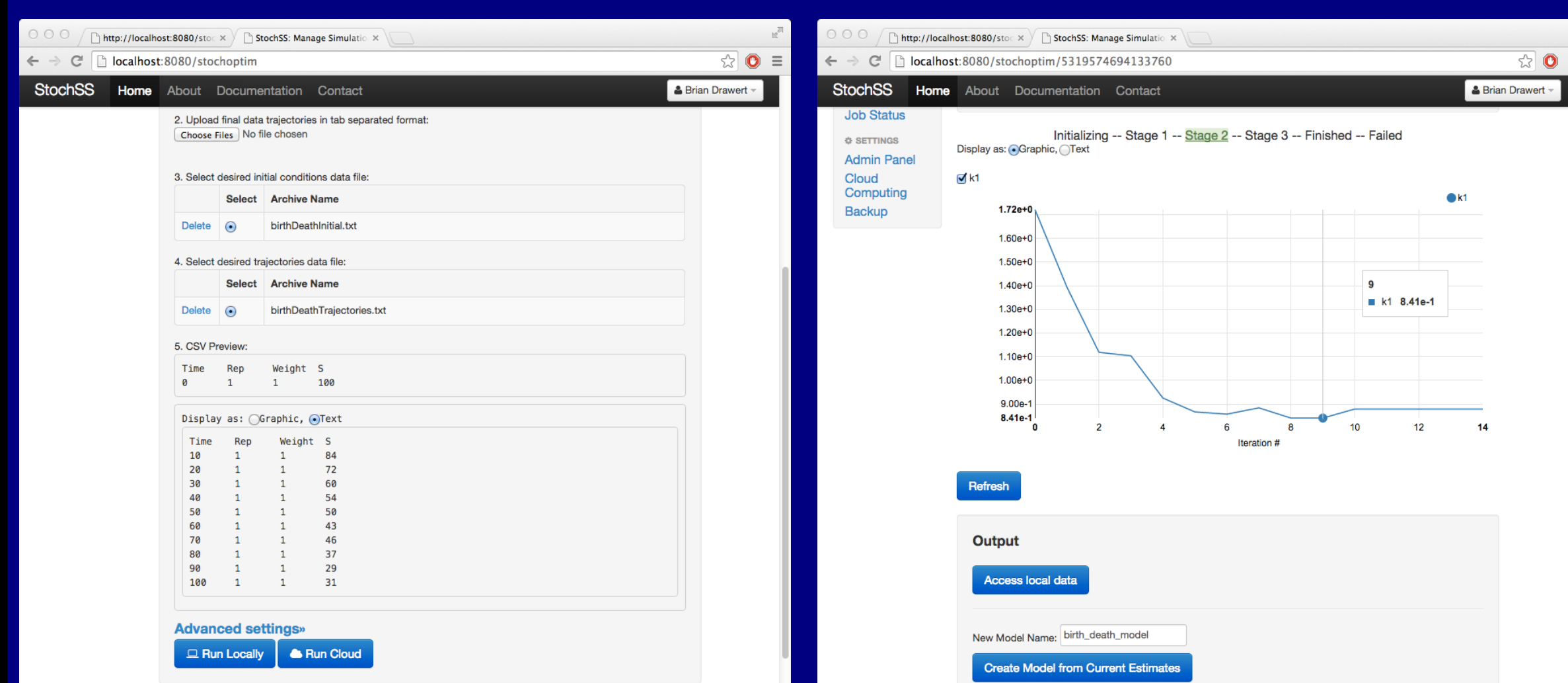
#### Run Simulations



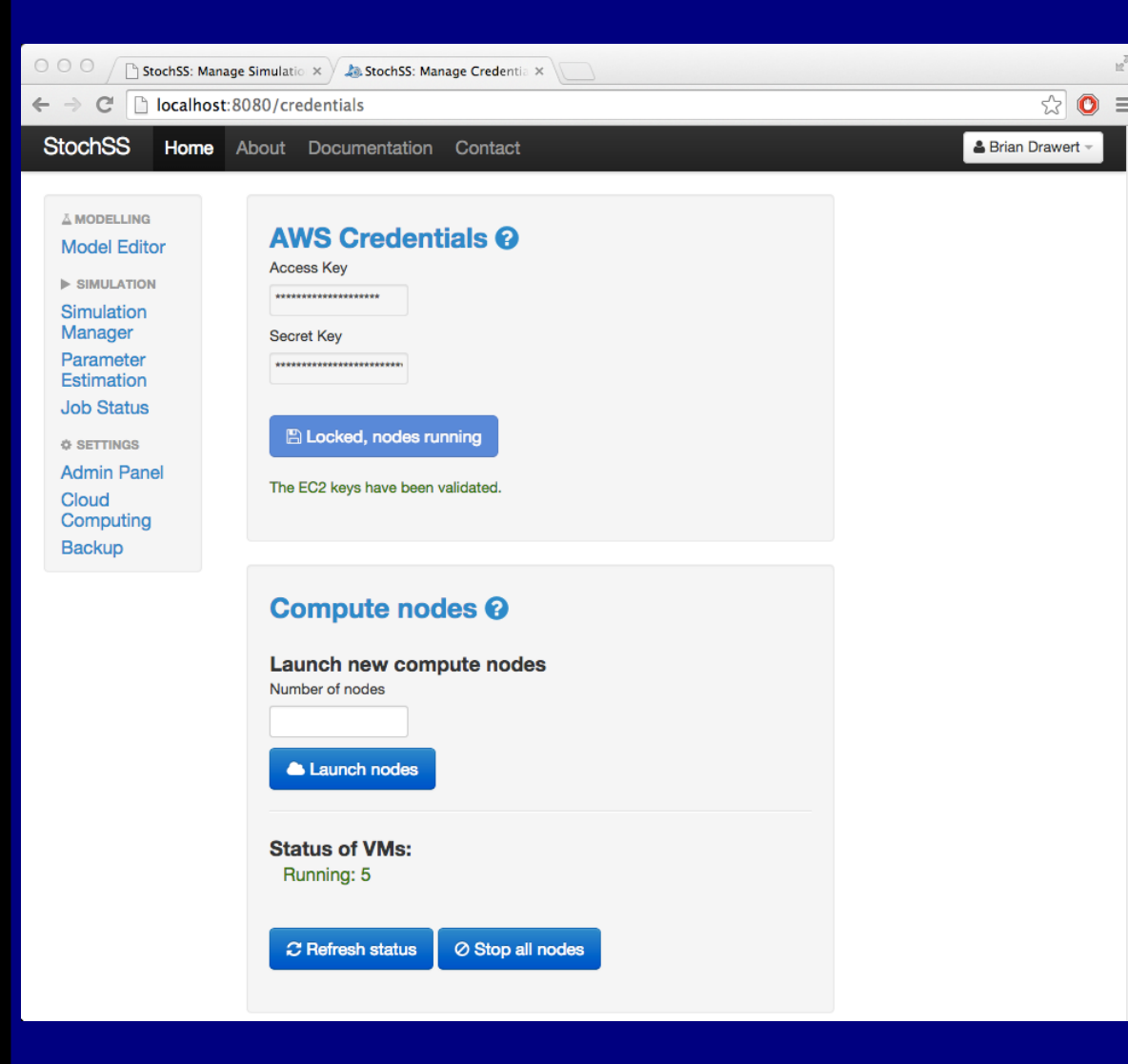
#### Visualize Results



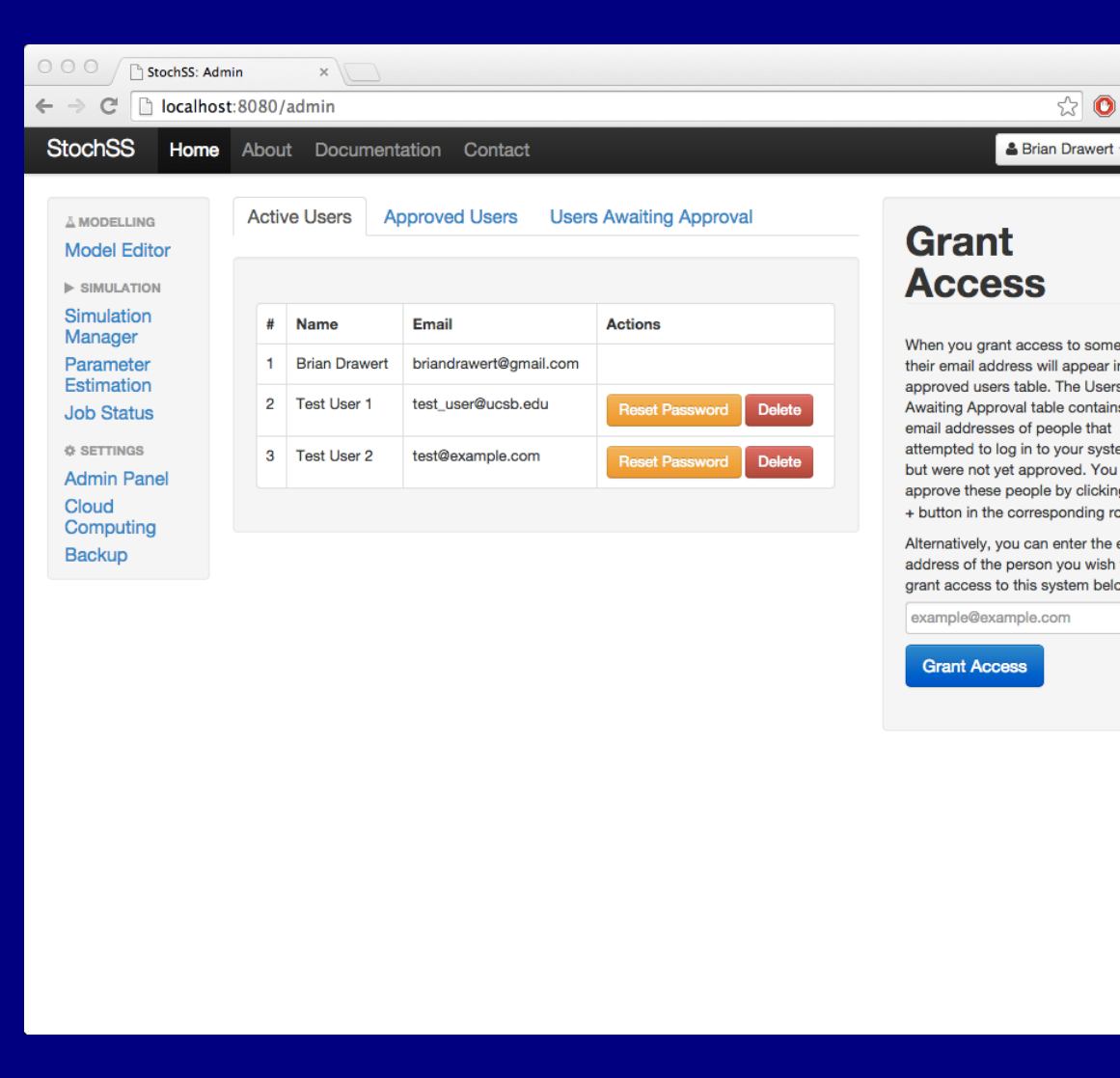
#### Estimate Parameters



#### Clusters On-Demand



#### Collaborate



### Our Vision

#### Build your Model

- StochSS provides an easy-to-use User Interface to quickly specify your model.
- Species, Parameters, Reactions, and Geometry.

#### Scale up the Complexity

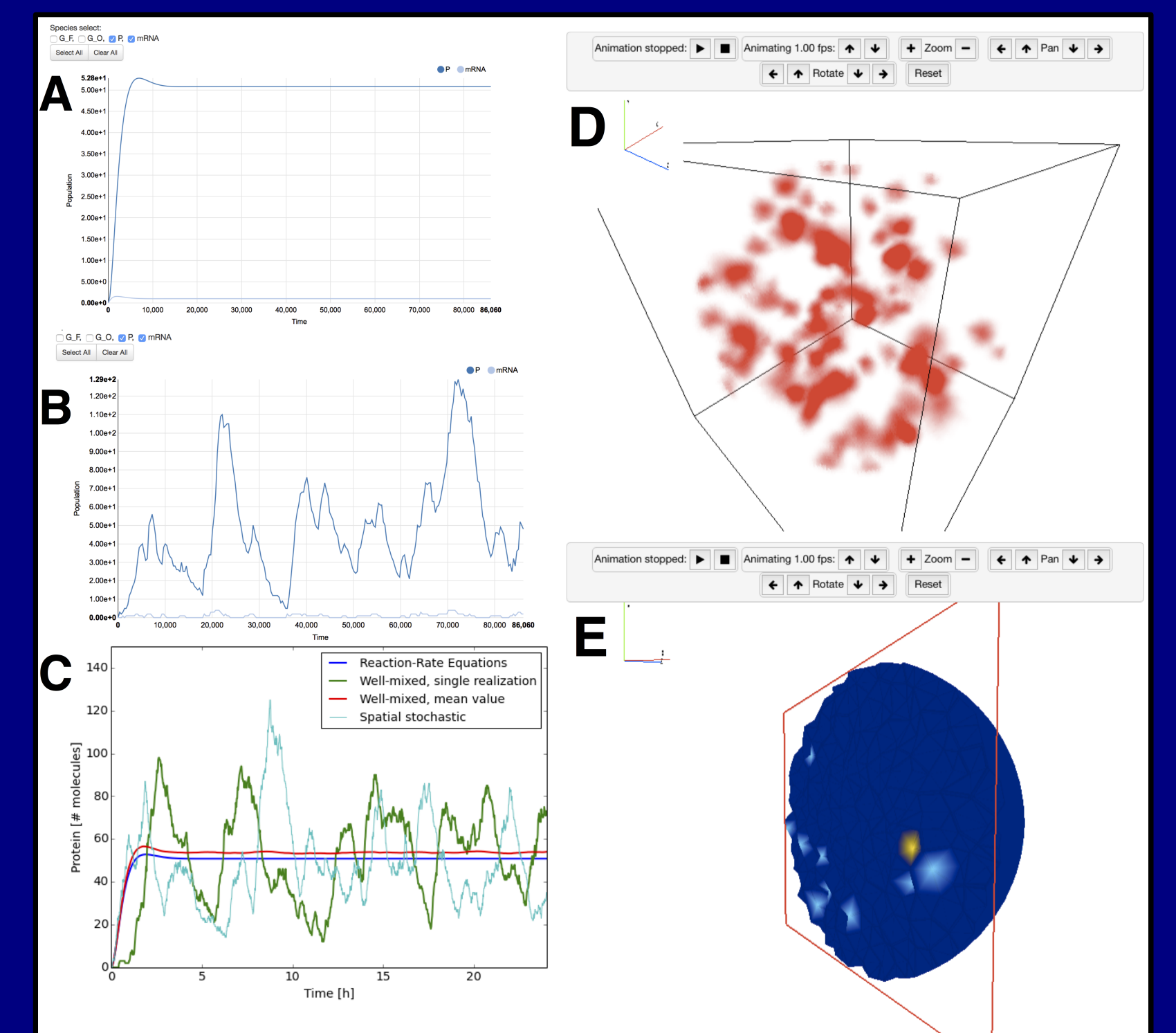
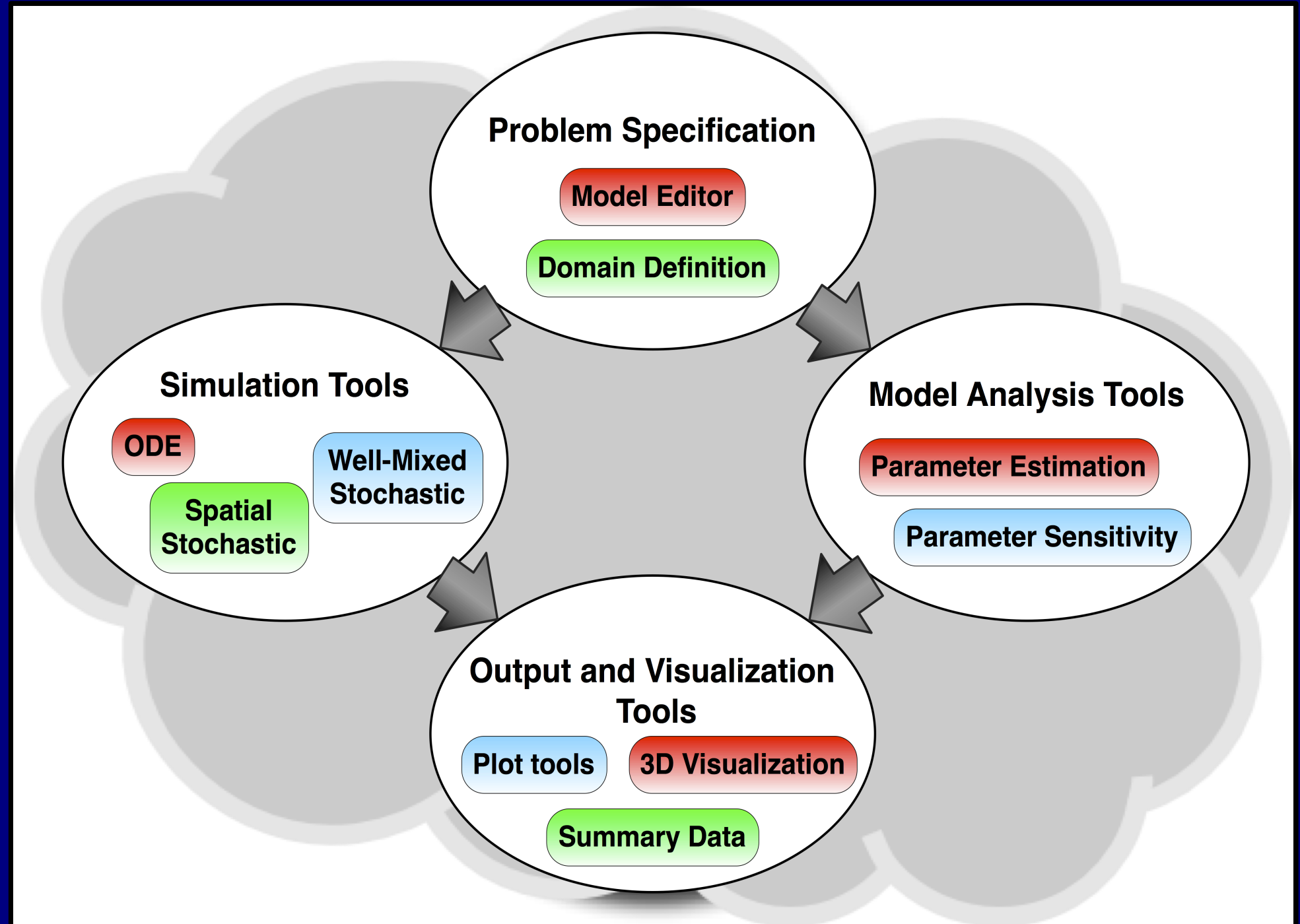
- In StochSS the same model can be used for multiple different types of simulation
- Deterministic (ODE) Simulation.
- Stochastic Simulation.
- Spatial Stochastic Simulation.
- Parameter Sensitivity.
- Estimation of Parameters from Data.

#### Clusters On-Demand

- Cloud Computing gives StochSS the ability to provide personal "Clusters On-Demand".
- Create a cluster with as much or as little computing power as you need, only when you need it.

#### Insight from Modeling

- StochSS provides state-of-the-art visualization of simulation results and easy methods to access and process data sets.



StochSS provides built-in visualization capabilities in order to quickly explore simulation results such as deterministic ODE simulations (A) and well-mixed discrete stochastic realizations (B). Key qualitative differences between the deterministic and stochastic simulations (C). Spatial stochastic simulations can be visualized and animated using volume rendering (D) and solid rendering with clipping (E).

### Roadmap

**StochSS v1.9 new release Apr 2017**  
Support for Batch Cluster Computing  
<http://try.stochss.org/> Test site for StochSS

**StochSS v1.8 released Oct 2016**  
Parameter Sweep tool allow 1D/2D sweeps  
Integrate Jupyter Notebooks for post-processing analysis