

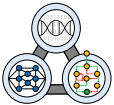
Hands On : Using MaBoSS with WebMaBoSS

Vincent Noël¹

¹Computational Systems Biology of Cancer,
Institut Curie, INSERM U900, Mines ParisTech, PSL Research University, Paris

Computational Systems Biology for Complex Human Disease
from static to dynamic representations of disease mechanisms

April 24th, 2024



Using MaBoSS with WebMaBoSS

› Home



WebMaBoSS

A web tool for simulating Boolean models

Click [here](#) to login if you already have an account, otherwise you can quickly create one [here](#).

If you want to quickly test WebMaBoSS, you can have a look at our [demo project](#).

Model analysis

WebMaBoSS allows simulations, and multiple outputs for results. It also allows sensitivity analysis by performing single and double mutations.

Compatibility

WebMaBoSS is able to import models in MaBoSS format (bnd, cfg files), BoolNet format, SBML-qual format, or in GINsim format. It also allows to export models in any of these three formats.

Public databases

WebMaBoSS allows to browse models from CellCollective and BioModels, and import them.

WebMaBoSS was created and is maintained by the team [Computational System Biology of Cancer](#) at [Institut Curie](#).


It is open-source and available on [GitHub](#), where you can also find instructions to run it locally and tutorials.

Using MaBoSS with WebMaBoSS

› Create an account

WebMaBoSS Tutorials About Demo Sign in Register

Register to WebMaBoSS



Username

E-mail (optional)

Password

Confirm password

[Register](#)

Using MaBoSS with WebMaBoSS

› Logging in



Sign in



Username

Password

[Sign in](#)

Using MaBoSS with WebMaBoSS

› List of projects

[WebMaBoSS](#) [Tutorials](#) [About](#) [Profile](#) [Logout](#)

Projects

Name	
Cell Cycle	✎ ✖
Metastasis	✎ ✖
Cell Fate	✎ ✖
Tutorial	✎ ✖
Cancer models	✎ ✖

New project

Using MaBoSS with WebMaBoSS

› Creating a project

The screenshot displays the WebMaBoSS web application. At the top, a dark navigation bar contains the text 'WebMaBoSS' followed by links for 'Tutorials' and 'About' on the left, and 'Profile' and 'Logout' on the right. The main content area has a dark header with the title 'Projects'. Below this, a list of existing projects is shown, each with a 'Name' label and a blue button: 'Cell Cycle', 'Metastasis', 'Cell Fate', 'Tutorial', and 'Cancer models'. A 'New project' button is located at the bottom left of this list. A modal window titled 'Add new project' is open in the center. It contains a 'Name' input field with the text 'Invasion models' and a 'Description' text area with the text 'Models describing invasion'. At the bottom of the modal are two buttons: a red 'Close' button and a blue 'Create project' button. On the right side of the background, a table lists the same five projects, each with a blue edit icon and a red delete icon.




Name	Description	Edit	Delete
Cell Cycle			
Metastasis			
Cell Fate			
Tutorial			
Cancer models			

Using MaBoSS with WebMaBoSS

› List of models

[WebMaBoSS](#) [Models](#) [Tutorials](#) [About](#) [Cancer models ▾](#) [Profile](#) [Logout](#)

Models

Name
Montagud 2021 Prostate Cancer   

[Load model](#) [Import model](#)

Using MaBoSS with WebMaBoSS

› Loading a model

The screenshot shows the WebMaBoSS interface with a 'Load model' dialog box open. The background interface includes a top navigation bar with 'WebMaBoSS', 'Models', 'Tutorials', and 'About'. On the right, there are links for 'Profile' and 'Logout'. The main content area is titled 'Models' and lists a model named 'Montagud 2021 Prostate Cancer'. Below this list are two buttons: 'Load model' and 'Import model'. The 'Load model' dialog box is a white modal with a title bar 'Load model'. It contains the following fields: 'Name' with the text 'Cohen 2015 Invasion model'; 'Type' with a dropdown menu showing 'MaBoSS'; 'BND file' with the text 'metastasis.bnd' and a 'Browse' button; and 'CFG file' with the text 'metastasis.cfg' and a 'Browse' button. At the bottom of the dialog are two buttons: a red 'Close' button and a blue 'Load model' button.

WebMaBoSS Models Tutorials About Profile Logout

Models

Name

Montagud 2021 Prostate Cancer

Load model Import model

Load model

Name

Cohen 2015 Invasion model

Type

MaBoSS

BND file

metastasis.bnd Browse

CFG file

metastasis.cfg Browse

Close Load model

Using MaBoSS with WebMaBoSS

› Importing a model

The screenshot shows the WebMaBoSS interface with the 'Import model' dialog box open. The dialog has two tabs: 'BioModels' and 'CellCollective'. The 'BioModels' tab is active, displaying a table of models. The table has two columns: 'Name' and 'Author'. The models listed are:

Name	Author
Traynard2016 - Mammalian cell cycle regulation - Logical Model	Pauline Traynard
Cacace2020 - Logical model of the regulatory network controlling...	Denis Thieffry
Howell2020- Compartmental Logical model of mitotic exit	Rowan Howell
Terfve2012 - Signalling in liver cancer - logical model	Vijayalakshmi Chelliah
Floc'hay2020 - SeaUrchin_model_ginsim	Denis Thieffry
Mbodj2016 - Mesoderm specification during Drosophila develop...	Denis Thieffry
Rodriguez-Jorge2019 - Boolean model of TCR signaling for CD4 +...	Denis Thieffry
Rodriguez-Jorge2019 - Boolean model of combined TCR and TLR...	Denis Thieffry
Afenya2018 - peripheral blood dynamics in the disease state	Szeyi Ng

At the bottom of the dialog, there is a toggle switch for 'Use SBML names' which is currently turned on, and a red 'Close' button.

Using MaBoSS with WebMaBoSS

› Model interaction graph



Using MaBoSS with WebMaBoSS

› Creating a new simulation : General settings

The screenshot shows the WebMaBoSS web application. The top navigation bar includes 'WebMaBoSS', 'Models', 'Tutorials', 'About', and 'Profile Logout'. The left sidebar has a dropdown menu for 'Cohen 2015 Invasion' and a list of options: 'Overview', 'Editing', 'Simulation', and 'Sensitivity'. The main content area displays 'Model Cohen 2015 Invasion' with a 'New simulation' button. A modal dialog box titled 'Create new simulation' is open, showing the 'General' tab. The dialog contains the following fields and controls:

- Name:** A text input field with the placeholder 'Name of the simulation'.
- Max time:** A numeric input field with the value '40'.
- Sample count:** A numeric input field with the value '1000'.
- Discrete time:** A toggle switch, currently turned off.
- Use physical random generator:** A toggle switch, currently turned off.
- Pseudorandom seed:** A numeric input field with the value '0'.

At the bottom of the dialog, there is a red 'Close' button and a 'Submit' button.

Using MaBoSS with WebMaBoSS

› Creating a new simulation : Initial states

The screenshot displays the WebMaBoSS web application interface. A modal dialog titled 'Create new simulation' is open, showing the 'Initial states' tab. The dialog lists several biological parameters with sliders and percentage values:

Parameter	Value
CTNNB1	0 %
CellCycleArrest	0 %
DKK1	0 %
DNA damage	50 %
ECMicroenv	50 %
EMT	0 %

At the bottom of the dialog, there are 'Close' and 'Submit' buttons. The background interface shows a sidebar with navigation links (Overview, Editing, Simulation, Sensitivity) and a main area with the title 'Model Cohen 2015 Inv...' and a 'New simulation' button.

Using MaBoSS with WebMaBoSS

› Creating a new simulation : Output nodes

The screenshot displays the WebMaBoSS web application interface. On the left, a sidebar contains navigation links: 'Cohen 2015 Invasion', 'Overview', 'Editing', 'Simulation', and 'Sensitivity'. The main content area shows the 'Model Cohen 2015 Invasion' with a 'New simulation' button. A modal dialog box titled 'Create new simulation' is open, featuring four tabs: 'General', 'Initial states', 'Output', and 'Mutations'. The 'Output' tab is active, showing a list of nodes with toggle switches: AKT1 (off), AKT2 (off), Apoptosis (on), CDH1 (off), CDH2 (off), CTNNB1 (off), and CellCycleArrest (on). At the bottom of the dialog are 'Close' and 'Submit' buttons.

Node	Status
AKT1	Off
AKT2	Off
Apoptosis	On
CDH1	Off
CDH2	Off
CTNNB1	Off
CellCycleArrest	On

Using MaBoSS with WebMaBoSS

› Creating a new simulation : Mutants

The screenshot displays the WebMaBoSS web application interface. A modal dialog titled 'Create new simulation' is open, showing the 'Mutations' tab. The dialog lists several biological components with toggle switches to enable or disable mutations for each. The 'AKT1' toggle is currently turned on (green), while the others are off (grey). At the bottom of the dialog are 'Close' and 'Submit' buttons.

WebMaBoSS Models Tutorials About Profile Logout

Cohen 2015 Invasion ~ Model Cohen 2015 Invasion

New simulation

Create new simulation

General Initial states Output Mutations

AKT1 ☒

AKT2 ☐

Apoptosis ☐

CDH1 ☐

CDH2 ☐

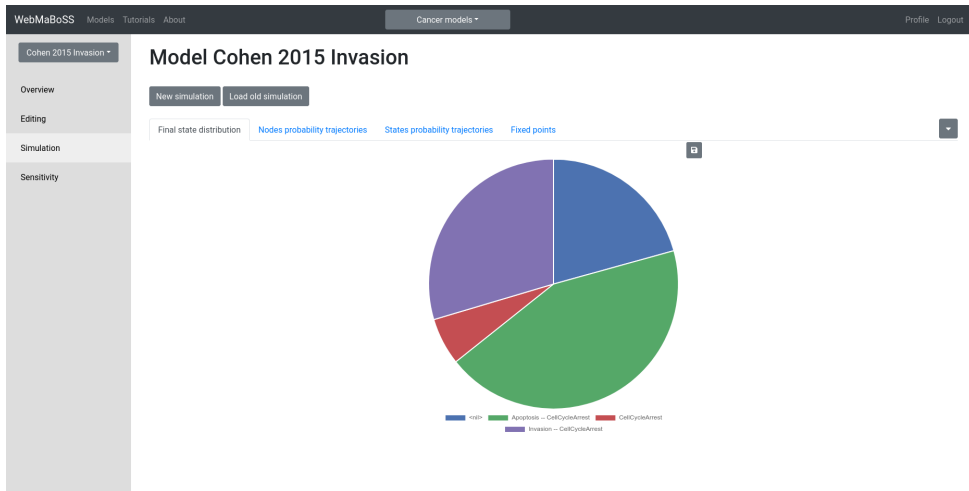
CTNNB1 ☐

CellPulseArrest ☐

Close Submit

Using MaBoSS with WebMaBoSS

› Simulation results : Final states



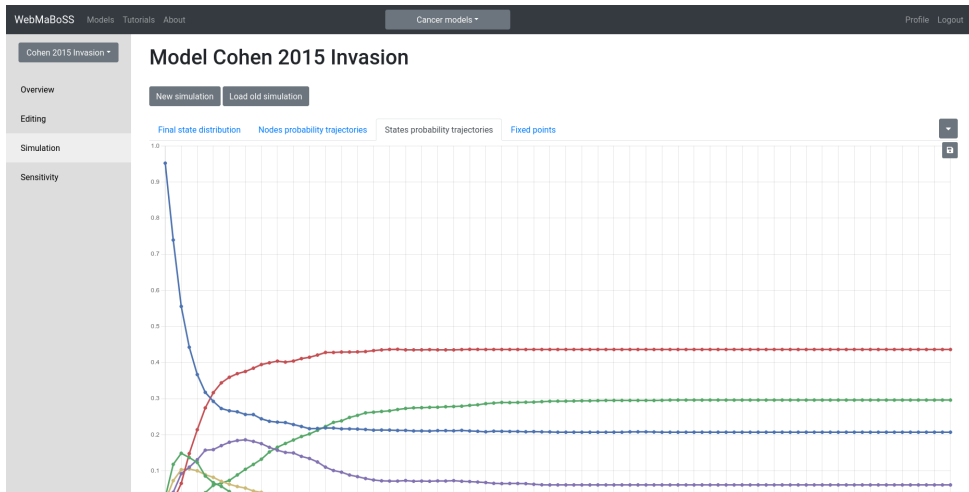
Using MaBoSS with WebMaBoSS

› Simulation results : Node trajectories



Using MaBoSS with WebMaBoSS

› Simulation results : State trajectories



- Simulation results : Fixed points



Using MaBoSS with WebMaBoSS

› Model editing : (in)activation rules

WebMaBoSS

ModelsTutorialsAbout

Cancer models ▾

ProfileLogout

Cohen 2015 Invasion ▾

Overview

Editing

Simulation

Sensitivity

Model Cohen 2015 Invasion

Rates

Initial values

Outputs

Parameters

Settings

AKT1		▾	▮
AKT2		▾	▮
Apoptosis		▾	▮
CDH1		▾	▮
CDH2		▾	▮
CTNNB1		▾	▮
CellCycleArrest		+	▮
rateUp	@logic ? \$u_CellCycleArrest : 0	▾	▮
rateDown	@logic ? 0 : \$d_CellCycleArrest	▾	▮
logic	(!p21 & !ZEB2 & !AKT1 & !miR200 & !miR203 & miR34) (!p21 & !ZEB2 & !AKT1 & !miR200 & miR203) (!p21 & !ZEB2 & !AKT1 & miR200) (!p21 & !ZEB2 & !AKT1) (p21 & !AKT1)	▾	▮
DKK1		▾	▮
DNA damage		▾	▮
ECMicroenv		▾	▮
EMT		▾	▮
ERK		▾	▮
GF		▾	▮
Invasion		▾	▮
Metastasis		▾	▮
Migration		▾	▮
NICD		▾	▮
SMAD		▾	▮
SNAI1		▾	▮

Using MaBoSS with WebMaBoSS

› Model editing : (in)activation rules

WebMaBoSS Models Tutorials About

Cohen 2015 Invasion

Overview Editing Simulation Sensitivity

Model Cohen 2015 Invasion

Rates Initial values Outputs Parameters

AKT1

AKT2

Apoptosis

CDH1

CDH2

CTNNB1

CellCycleArrest

rateUp @logic ? \$u_CellCycleArrest : 0

rateDown @logic ? 0 : \$d_CellCycleArrest

logic (!p21 & !ZEB2 & !AKT1 & !miR200 & !miR203 & miR34) | (!p21 & !ZEB2 & !AKT1 & !miR200 & !miR203) | (!p21 & !ZEB2 & !AKT1 & miR200) | (!p21 & ZEB2 & !AKT1) | (p21 & !AKT1)

DKK1

DNA damage

ECMicroenv

EMT

ERK

GF

Invasion

Metastasis

Migration

NICD

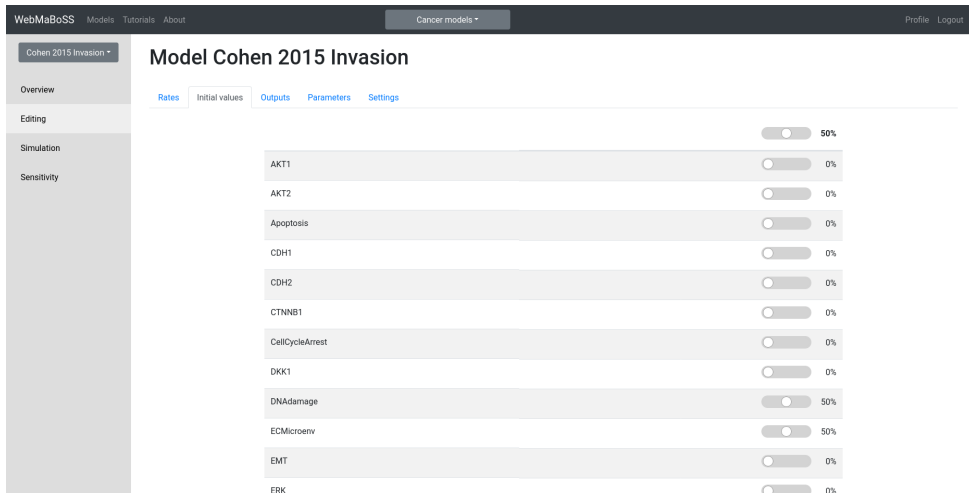
SMAD

SNAIL

Close Submit

Using MaBoSS with WebMaBoSS

› Model editing : Initial states



The screenshot shows the WebMaBoSS web application interface. The top navigation bar includes 'WebMaBoSS', 'Models', 'Tutorials', 'About', a 'Cancer models' dropdown, and 'Profile' and 'Logout' links. The left sidebar contains a 'Cohen 2015 Invasion' dropdown and a list of tabs: 'Overview', 'Editing', 'Simulation', and 'Sensitivity'. The main content area is titled 'Model Cohen 2015 Invasion' and has sub-tabs for 'Rates', 'Initial values', 'Outputs', 'Parameters', and 'Settings'. The 'Initial values' tab is active, displaying a list of biological entities with their initial state percentages.

Entity	Initial Value (%)
AKT1	50%
AKT2	0%
Apoptosis	0%
CDH1	0%
CDH2	0%
CTNNB1	0%
CellCycleArrest	0%
DKK1	0%
DNA damage	50%
ECMicroenv	50%
EMT	0%
ERK	0%

Using MaBoSS with WebMaBoSS

› Model editing : Output nodes

The screenshot displays the WebMaBoSS web application interface. At the top, a dark navigation bar contains the 'WebMaBoSS' logo, links for 'Models', 'Tutorials', and 'About', a 'Cancer models' dropdown menu, and 'Profile' and 'Logout' links. On the left, a sidebar shows a 'Cohen 2015 Invasion' dropdown and a list of navigation options: 'Overview', 'Editing', 'Simulation', and 'Sensitivity'. The main content area is titled 'Model Cohen 2015 Invasion' and features four tabs: 'Rates', 'Initial values', 'Outputs' (which is active), and 'Parameters'. Below the tabs, a list of output nodes is shown, each with a toggle switch. The nodes and their states are: AKT1 (off), AKT2 (off), Apoptosis (on), CDH1 (off), CDH2 (off), CTNNB1 (off), CellCycleArrest (on), DKK1 (off), DNADamage (off), ECMicroenv (off), EMT (off), ERK (off), GF (off), and Invasion (on).

Output Node	Toggle State
AKT1	Off
AKT2	Off
Apoptosis	On
CDH1	Off
CDH2	Off
CTNNB1	Off
CellCycleArrest	On
DKK1	Off
DNADamage	Off
ECMicroenv	Off
EMT	Off
ERK	Off
GF	Off
Invasion	On

Using MaBoSS with WebMaBoSS

› Model editing : Parameters

WebMaBoSS

ModelsTutorialsAbout

Cancer models ▾

ProfileLogout

Cohen 2015 Invasion ▾

Overview

Editing

Simulation

Sensitivity

Model Cohen 2015 Invasion

RatesInitial valuesOutputsParametersSettings

\$d_AKT1	1		
\$d_AKT2	1		
\$d_Apoptosis	1		
\$d_CDH1	1		
\$d_CDH2	1		
\$d_CTNNB1	1		
\$d_CellCycleArrest	1		
\$d_DKK1	1		
\$d_DNADamage	1		
\$d_ECMicroenv	1		
\$d_EMT	1		
\$d_ERK	1		
\$d_GF	1		
\$d_Invasion	1		
\$d_Metastasis	1		
\$d_Migration	1		
\$d_NICD	1		
\$d_SMAD	1		
\$d_SNAI1	1		
\$d_SNAI2	1		
\$d_TGFbeta	1		

Using MaBoSS with WebMaBoSS

› Model editing : Settings

WebMaBoSS

Models

Tutorials

About

Cancer models ▾

Profile

Logout

Cohen 2015 Invasion ▾

Overview












Editing

Simulation

Sensitivity

Model Cohen 2015 Invasion

[Rates](#)[Initial values](#)[Outputs](#)[Parameters](#)[Settings](#)

time_tick	0.5	
max_time	40	
sample_count	1000	
discrete_time	0	
use_physrandgen	0	
seed_pseudorandom	0	
display_traj	0	
statdist_traj_count	0	
statdist_cluster_threshold	1	
thread_count	6	
statdist_similarity_cache_max_size	20000	

Using MaBoSS with WebMaBoSS

› Sensitivity analysis : General settings

The screenshot displays the WebMaBoSS web application interface. At the top, a dark navigation bar contains the text 'WebMaBoSS' and links for 'Models', 'Tutorials', 'About', 'Profile', and 'Logout'. On the left, a sidebar lists navigation options: 'Cohen 2015 Invasion', 'Overview', 'Editing', 'Simulation', and 'Sensitivity'. The main content area is titled 'Model Cohen 2015 Invasion' and includes a 'New sensitivity analysis' button. A modal dialog box titled 'New sensitivity analysis' is open in the center. It features three tabs: 'General' (selected), 'Candidates', and 'Output'. The 'General' tab contains a 'Name' field with the placeholder 'Name of the simulation', two toggle switches for 'Single mutations' and 'Double mutations' (both currently turned off), and a 'Local' dropdown menu. At the bottom of the dialog are 'Close' and 'Submit' buttons.

Using MaBoSS with WebMaBoSS

› Sensitivity analysis : Mutant candidates

The screenshot displays the WebMaBoSS web application. The main interface is dark-themed with a sidebar on the left containing navigation links: Overview, Editing, Simulation, and Sensitivity. The top navigation bar includes 'WebMaBoSS', 'Models', 'Tutorials', 'About', 'Profile', and 'Logout'. The main content area shows 'Model Cohen 2015 Inv' with a 'New sensitivity analysis' button. A modal window titled 'New sensitivity analysis' is open, featuring three tabs: 'General', 'Candidates', and 'Output'. The 'Candidates' tab is active, showing a list of biological processes with toggle switches: ERK (on), GF (on), Invasion (off), Metastasis (off), Migration (off), and NICD (on). At the bottom of the modal are 'Close' and 'Submit' buttons.

Process	Toggle State
ERK	On
GF	On
Invasion	Off
Metastasis	Off
Migration	Off
NICD	On

Using MaBoSS with WebMaBoSS

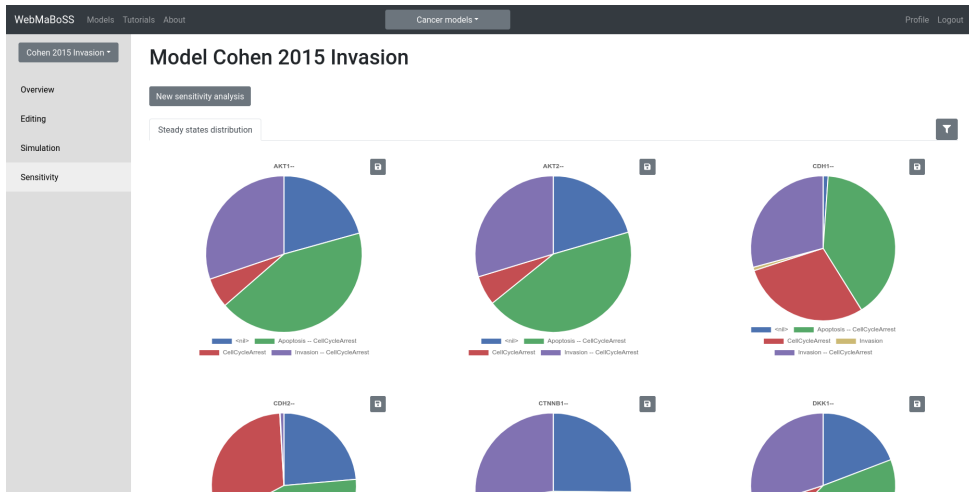
› Sensitivity analysis : Output nodes

The screenshot displays the WebMaBoSS web application interface. On the left, a sidebar contains navigation links: Overview, Editing, Simulation, and Sensitivity. The main content area shows the 'Model Cohen 2015 Invasion' with a 'New sensitivity analysis' button. A modal dialog box titled 'New sensitivity analysis' is open, featuring three tabs: General, Candidates, and Output. The 'Output' tab is active, showing a list of nodes with toggle switches. The nodes and their states are: AKT1 (off), AKT2 (off), Apoptosis (on), CDH1 (off), CDH2 (off), and CTNNB1 (off). At the bottom of the dialog are 'Close' and 'Submit' buttons.

Node	State
AKT1	Off
AKT2	Off
Apoptosis	On
CDH1	Off
CDH2	Off
CTNNB1	Off

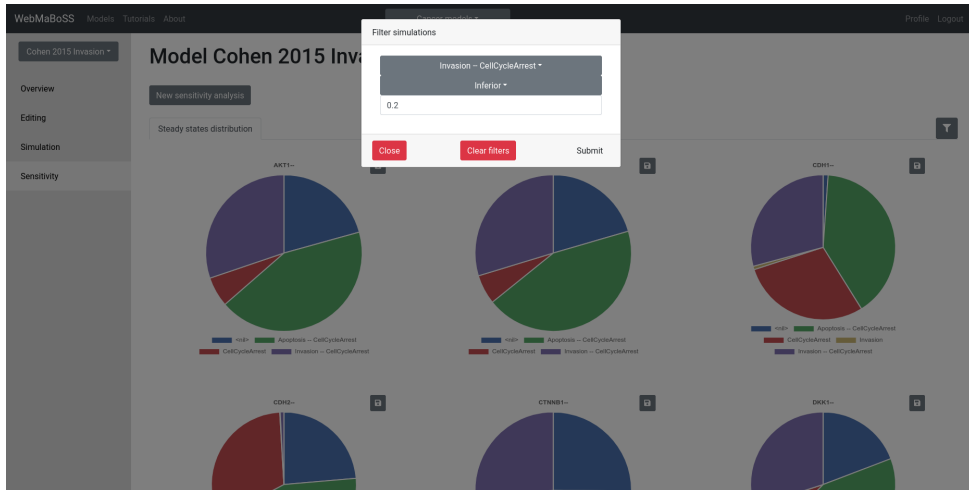
Using MaBoSS with WebMaBoSS

› Sensitivity analysis : Results



Using MaBoSS with WebMaBoSS

› Sensitivity analysis : Filtering results



Using MaBoSS with WebMaBoSS

› Sensitivity analysis : Filtered results



Using MaBoSS with WebMaBoSS

- › Hands on

- › Create a new project
- › Load Cohen's model (bnd and cfg available in manuals/Modules/MaBoss/ folder)
- › Perform default simulation
- › Perform simulation with ECMicroenv and DNADamage on

Using MaBoSS with WebMaBoSS

- › Hands on

- › Perform simulation with NICD++, p53– mutant
- › Perform sensitivity analysis on single mutants, testing only inhibitions
- › Filter mutants where state Invasion – CellCycleArrest is less than 20%