Introduction to Dynamical Models in Biology
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Lecture 07
Introduction to JSim

Hello, welcome to the second week of our course on dynamical modules in biology. This is module 1. In last few modules we have discussed about analytical method and numerical method of solving ordinary differential equation based models. In this module and the subsequent one we will discuss about different software or tools available to you for solving ordinary differential based models using numerical methods. Particularly I will focus on one freely available software called JSim that you can use to solve ordinary differential based models. So let us look into different options that you have at hand to simulate ordinary differential equation based models using some programming language or by using some readymade software.

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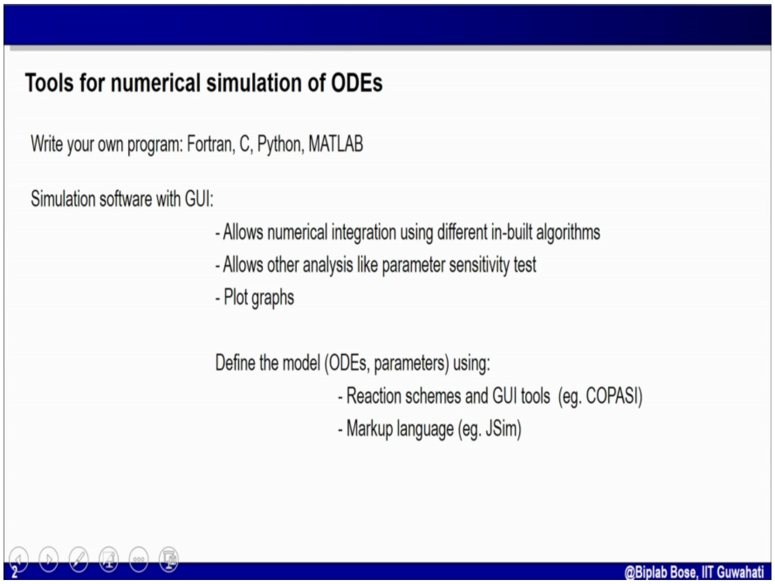

Tools for numerical simulation of ODEs

Write your own program: Fortran, C, Python, MATLAB

Simulation software with GUI:

- Allows numerical integration using different in-built algorithms
- Allows other analysis like parameter sensitivity test
- Plot graphs

Define the model (ODEs, parameters) using:

- Reaction schemes and GUI tools (eg. COPASI)
- Markup language (eg. JSim)

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There are many programming languages starting of Fortran, C, Python that you can use depending upon your experience and ease to write your own code to solve a ordinary differential equation based model. Either you can use higher level languages like MATLAB for that. Most of these languages has inbuilt library function for solving ODE numerically and different algorithms are available. If you are not comfortable with using in writing program for yourself you can look for readymade software which is Plug and Play and you can use them to solve your model. Now these softwares are actually GUI based. They have a graphic user interface which helps you to analyze the model with ease.

Some of these GUI can have the option where you can simply write down the equation and ask the system to simulate the model. In some cases you have to use a particular markup language that is understood by the software to define the model. Depending upon your choice you will use one of them. For example software like COPASI, these are the software where you can define a reaction just like $A+B \rightarrow C$ like this whereas JSIM that we will learn, we will have to define the model using a specific manner, using a specific language that JSIM will understand.

Now all of these software have certain advantages, most of them have multiple algorithm available with them so that you can choose one of the algorithm based on your utility. They not only allow you to solve ODE but they also have certain other tools for example parameter estimation, parameter sensitivity analysis, we will not discuss those but those tools are many times very useful. The last importance of GUI based stimulation software is that most of them has readymade visualization or plotter with it. So once you simulate it the graph for the dependent variable comes up automatically. So you can visualize the simulation immediately and you won’t have to use a separate plotter or grapher tool for plotting tour data. With these let us start and look into the different aspect of JSIM, a java based simulation software that we will use for our work.

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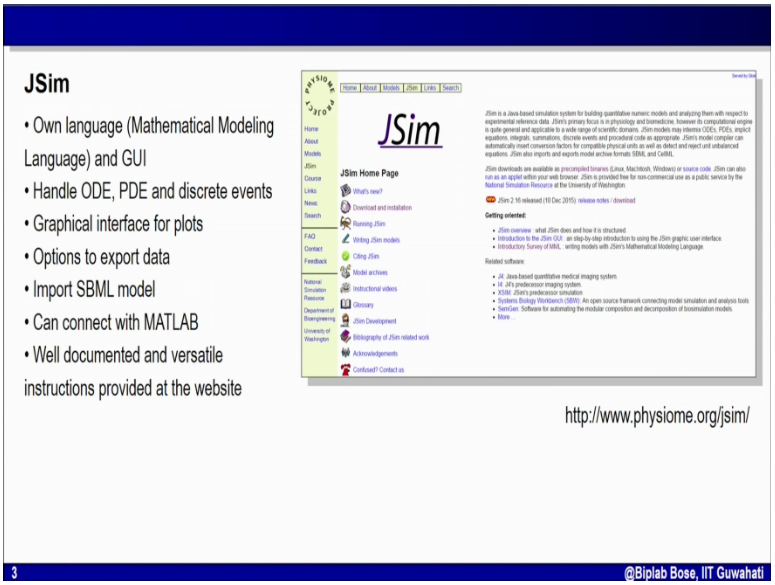

JSim

- Own language (Mathematical Modeling Language) and GUI
- Handle ODE, PDE and discrete events
- Graphical interface for plots
- Options to export data
- Import SBML model
- Can connect with MATLAB
- Well documented and versatile instructions provided at the website

JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also imports and exports model archive formats SBML and CellML.

JSim downloads are available as precompiled binaries (Linux, Macintosh, Windows) or source code. JSim can also run as an applet within your web browser. JSim is provided free for non-commercial use as a public service by the National Simulation Resource at the University of Washington.

JSim 2.16 released (10 Dec 2015): release notes / download

Getting oriented:

- JSim overview : what JSim does and how it is structured.
- Introduction to the JSim GUI : an step-by-step introduction to using the JSim graphic user interface.
- Introductory Survey of MML : writing models with JSim's Mathematical Modeling Language.

Related software:

- J4: Java-based quantitative medical imaging system.
- I4: J4's predecessor imaging system.
- XSIM: JSim's predecessor simulation.
- Systems Biology Workbench (SBW): An open source framwork connecting model simulation and analysis tools
- SemGen: Software for automating the modular composition and decomposition of biosimulation models.
- More ...

http://www.physiome.org/jsim/

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JSim is freely available. You can download from a web, the address are given here, www.fisium.org/JSim. As I have said JSim is GUI based software but it requires you to write down the model in its own language. So this language is called mathematical modeling language. Interestingly JSim can handle ordinary differential equation, it can handle partial differential equation and even it can model with discrete event. It has graphical user interface where you can plot data and your result. It has option to export your data as text file so that you can plot the graphs in some other software like Microsoft XL. It can import SBNL model. SBML stands for System Biology Markup Language.

As you know dynamical models are very common in system biology and different people use different language and different software to simulate this model. That is why scientists are trying to develop a common markup language that will be used by everybody working in the field of system biology. System Biology Markup Language is one such effort, one such markup language and interestingly JSim can export-import its model in SBML format. You can also connect JSim with MATLAB, that is very powerful option you have and the best part of JSim is that at website you have well documented tutorials. You have videos, you have text tutorials, you have large number of modules available there through which you can learn. So learning JSim is much easier.

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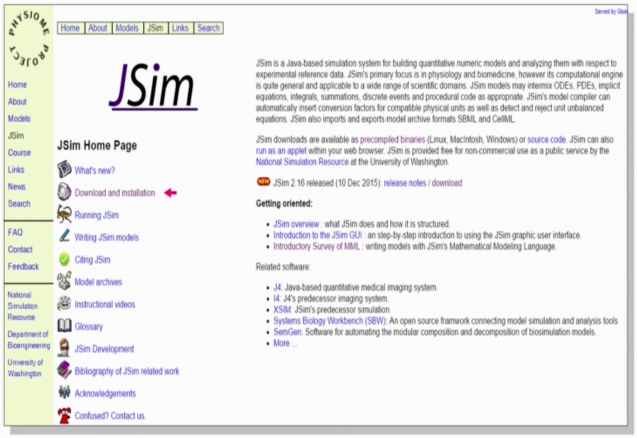
Download JSim



JSim Home Page

- What's new?
- Download and installation
- Running JSim
- Writing JSim models
- Citing JSim
- Model archives
- Instructional videos
- Glossary
- JSim Development
- Bibliography of JSim related work
- Acknowledgements
- Confused? Contact us.

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NEW JSim 2.16 released (10 Dec 2015): release notes / download

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- XSIM: JSim's predecessor simulation
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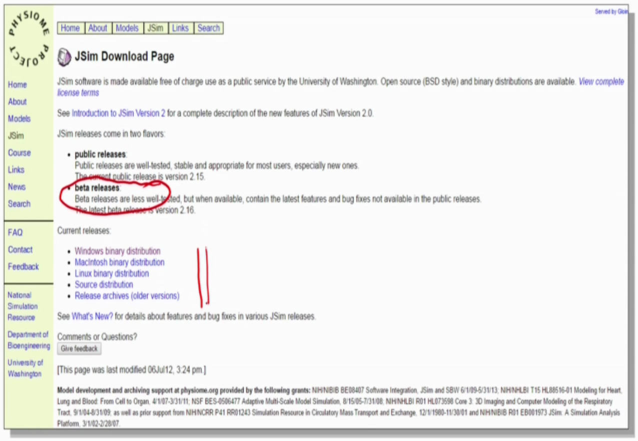
- More ...

Download JSim



JSim Download Page

JSim software is made available free of charge use as a public service by the University of Washington. Open source (BSD style) and binary distributions are available. *View complete license terms*

See Introduction to JSim Version 2 for a complete description of the new features of JSim Version 2.0.

JSim releases come in two flavors:

- **public releases**:
  Public releases are well-tested, stable and appropriate for most users, especially new ones.
  The current public release is version 2.15.
- **beta releases**:
  Beta releases are less well-tested, but when available, contain the latest features and bug fixes not available in the public releases.
  The latest beta release is version 2.16.

Current releases:

- Windows binary distribution
- Macintosh binary distribution
- Linux binary distribution
- Source distribution
- Release archives (older versions)

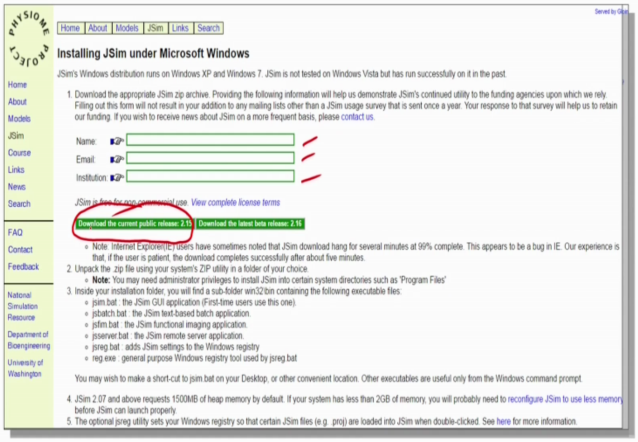
See What's New? for details about features and bug fixes in various JSim releases.

Comments or Questions?
Give feedback

[This page was last modified 06Jul12, 3:24 pm.]

Model development and archiving support at physiome.org provided by the following grants: NIH/NIBIB BE08407 Software Integration, JSim and SBW 6/1/09-5/31/13; NIH/NHLBI T15 HL88516-01 Modeling for Heart, Lung and Blood: From Cell to Organ, 4/1/07-3/31/11; NSF BES-0506477 Adaptive Multi-Scale Model Simulation, 8/15/05-7/31/08; NIH/NHLBI R01 HL073598 Core 3: 3D Imaging and Computer Modeling of the Respiratory Tract, 9/1/04-8/31/09; as well as prior support from NIH/NCRR P41 RR01243 Simulation Resource in Circulatory Mass Transport and Exchange, 12/1/1980-11/30/01 and NIH/NIBIB R01 EB001973 JSim: A Simulation Analysis Platform, 3/1/02-2/28/07.

Download JSim



Home | About | Models | JSim | Links | Search

Served by Gl...

Installing JSim under Microsoft Windows

JSim's Windows distribution runs on Windows XP and Windows 7. JSim is not tested on Windows Vista but has run successfully on it in the past.

1. Download the appropriate JSim zip archive. Providing the following information will help us demonstrate JSim's continued utility to the funding agencies upon which we rely. Filling out this form will not result in your addition to any mailing lists other than a JSim usage survey that is sent once a year. Your response to that survey will help us to retain our funding. If you wish to receive news about JSim on a more frequent basis, please contact us.

   Name: ✓

   Email: ✓

   Institution: ✓

   JSim is free for non-commercial use. View complete license terms

   Download the current public release: 2.15 | Download the latest beta release: 2.16

   - Note: Internet Explorer(IE) users have sometimes noted that JSim download hang for several minutes at 99% complete. This appears to be a bug in IE. Our experience is that, if the user is patient, the download completes successfully after about five minutes.
2. Unpack the .zip file using your system's ZIP utility in a folder of your choice.
   - **Note:** You may need administrator privileges to install JSim into certain system directories such as 'Program Files'
3. Inside your installation folder, you will find a sub-folder win32\bin containing the following executable files:
   - jsim.bat : the JSim GUI application (First-time users use this one).
   - jsbatch.bat : the JSim text-based batch application.
   - jsfim.bat : the JSim functional imaging application.
   - jsserver.bat : the JSim remote server application.
   - jsreg.bat : adds JSim settings to the Windows registry
   - reg.exe : general purpose Windows registry tool used by jsreg.bat

   You may wish to make a short-cut to jsim.bat on your Desktop, or other convenient location. Other executables are useful only from the Windows command prompt.
4. JSim 2.07 and above requests 1500MB of heap memory by default. If your system has less than 2GB of memory, you will probably need to reconfigure JSim to use less memory before JSim can launch properly.
5. The optional jsreg utility sets your Windows registry so that certain JSim files (e.g. .proj) are loaded into JSim when double-clicked. See here for more information.

The first thing you should do is go to JSim website and download it. You have a link here to download JSim. When you click you go to the download page. In download page you have options for choosing right JSimM. For example if you are using windows system use windows binary distribution, if you are using a Linux machine you download the Linux one. Once you are there you have to fill up this form which is very brief. Put your name, email and institution name and then download it from this click. You can download the Beta version but to begin with I will recommend not downloading the beta version but using the current public reviews.

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Using JSim

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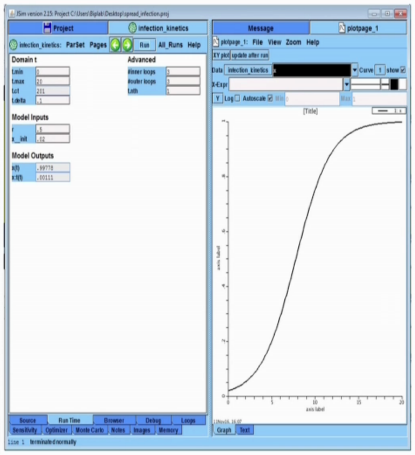


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj

Domain t

t.min 0

t.max 20

t.ct 201

t.delta .1

Advanced

#inner loops 3

#outer loops 3

t.nth 1

Model Inputs

r .5

x_init .02

Model Outputs

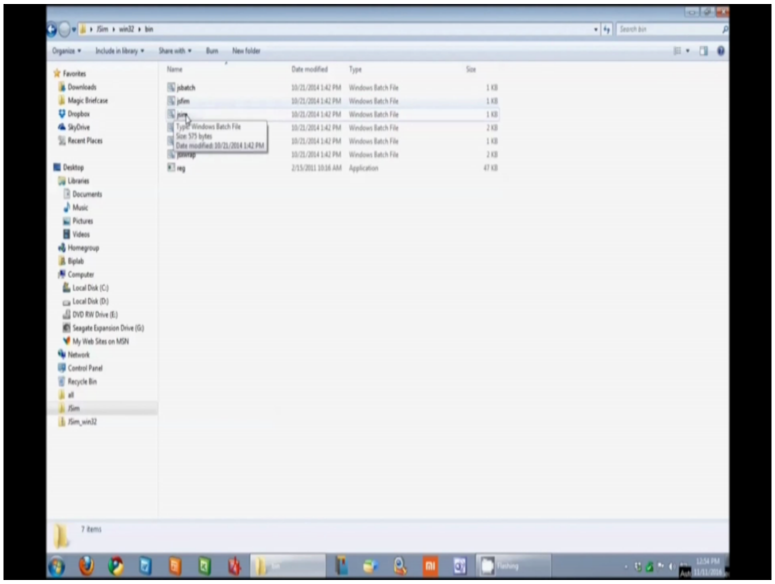
x(t) .99778

x:t(t) .00111

Data infection_kinetics x | Curve 1 | show ☑

Y | Log □ | Autoscale ☑ | Min 0 | Max 1

line 1 terminated normally



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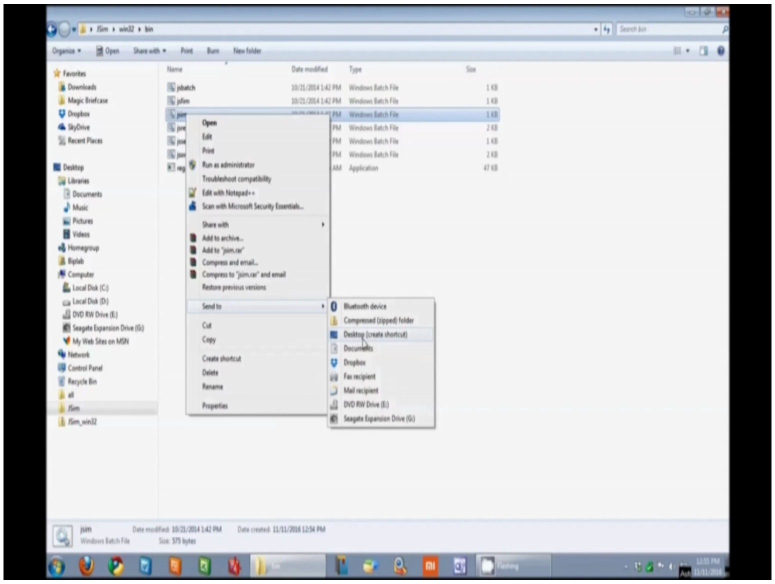
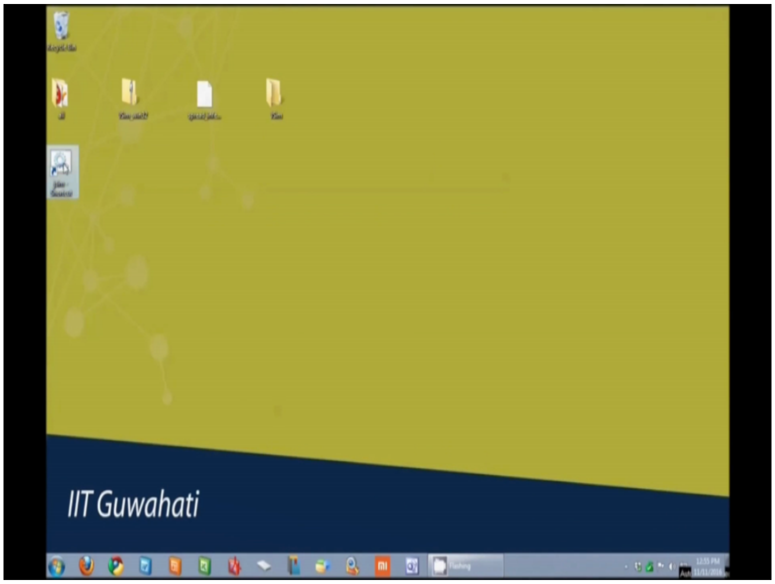
jsfim	10/21/2014 1:42 PM	Windows Batch File	1 KB
jsim	10/21/2014 1:42 PM	Windows Batch File	1 KB
[illegible]	10/21/2014 1:42 PM	Windows Batch File	2 KB
[illegible]	10/21/2014 1:42 PM	Windows Batch File	1 KB
jswrap	10/21/2014 1:42 PM	Windows Batch File	2 KB
reg	2/15/2011 10:16 AM	Application	47 KB

Type: Windows Batch File
Size: 575 bytes
Date modified: 10/21/2014 1:42 PM

7 items



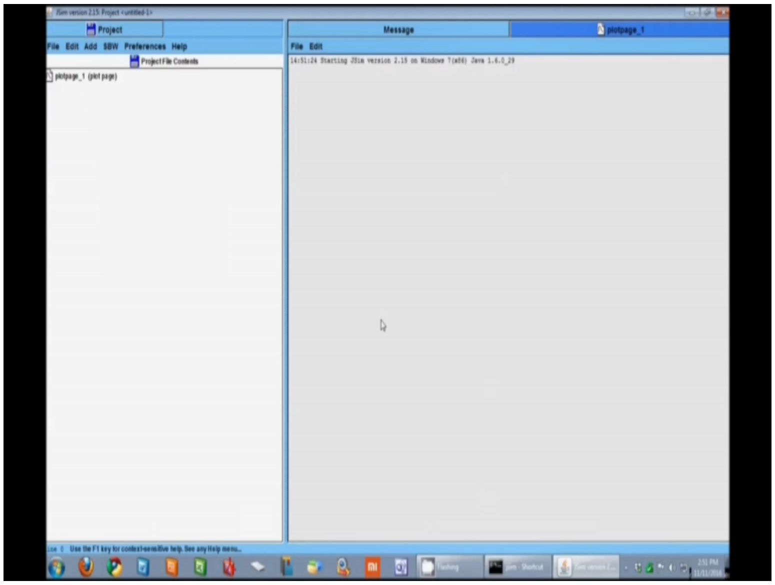
jsim Date modified: 10/21/2014 1:42 PM Date created: 11/11/2016 12:54 PM
Windows Batch File Size: 575 bytes



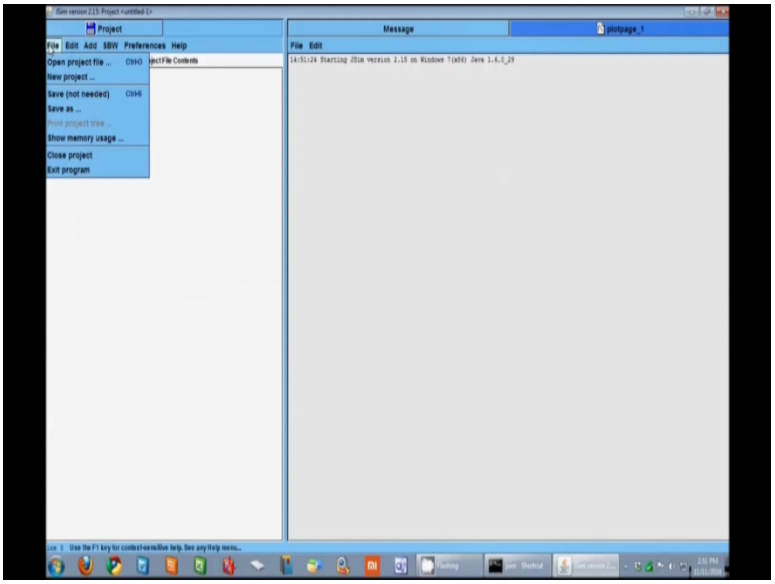
Once you have downloaded it you are ready to go and simulate some model. Let us try some video which I have recorded and to show how you can use JSim. I have downloaded the Windows version. It is a zip file, I have to unzip and uncompress it, so let us extract it here. The files will be extracted on my desktop. Wait for few seconds. Okay! Extraction is over. I want to put all these files in a particular folder. Let us name it JSim and put all these extracted files in this folder. You can keep this folder in some other directory for example in program directory. Go to this folder now.

Once you open, you can see some other sub folders are there. We are interested in this Win32 folder. In that you have again 4 folders. Open the bin. Now in this bin you have lots of Windows batch files. We are interested in running that JSim batch file, so we will make a shortcut of that to desktop so that every time I click on that shortcut, JSim will start. Close this window. Here you have. You have the shortcut for JSim on your desktop now. It is very easy to use, you double click on it and JSim will start.

(Refer Slide Time: 8:55)


JSim version 2.15: Project <untitled-1>
Project
File Edit Add SBW Preferences Help
Project File Contents
plotpage_1 (plot page)
Message
plotpage_1
File Edit
Use the F1 key for context-sensitive help. See any Help menu.

```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
```



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14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
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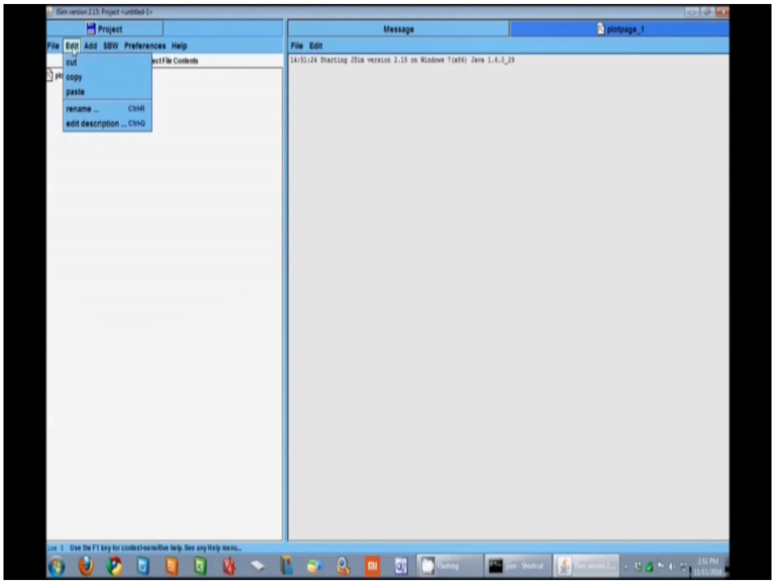

JSim version 2.15: Project <untitled-1>
Project
File
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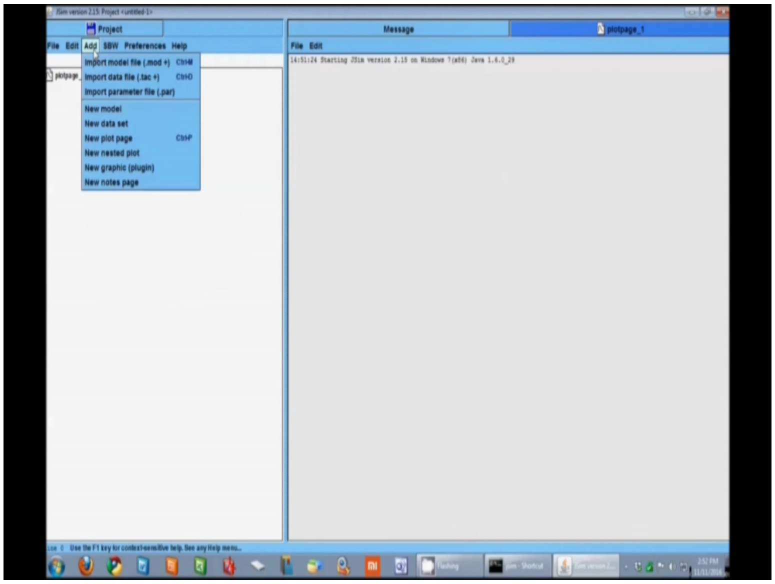
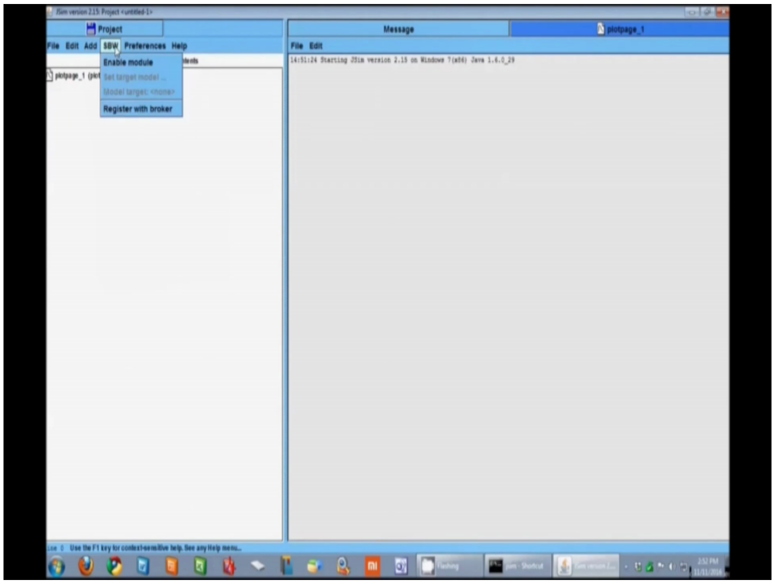
rename ... Ctrl-R
edit description ... Ctrl-G
Project File Contents
Message
plotpage_1
File
Edit
Use the F1 key for context-sensitive help. See any Help menu...

```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
```

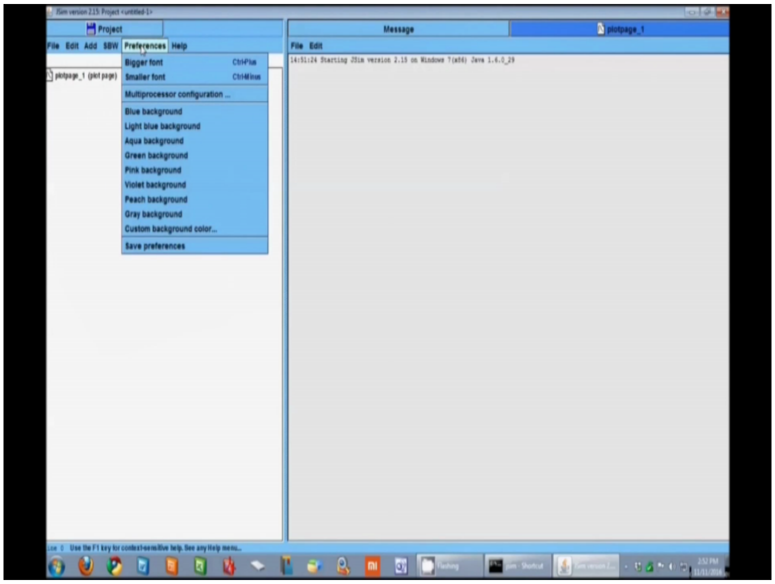


JSim version 2.15: Project <untitled-1>
Project
File
Edit
Add
SBW
Preferences
Help
Import model file (.mod +) Ctrl-M
Import data file (.tac +) Ctrl-D
Import parameter file (.par)
New model
New data set
New plot page Ctrl-P
New nested plot
New graphic (plugin)
New notes page
plotpage_
Message
plotpage_1
File
Edit
Use the F1 key for context-sensitive help. See any Help menu...

```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
```


JSim version 2.15: Project <untitled-1>
Project
File Edit Add SBW Preferences Help
Enable module
Set target model ...
Model target: <none>
Register with broker
plotpage_1 (plot
Message
plotpage_1
File Edit
Use the F1 key for context-sensitive help. See any Help menu...

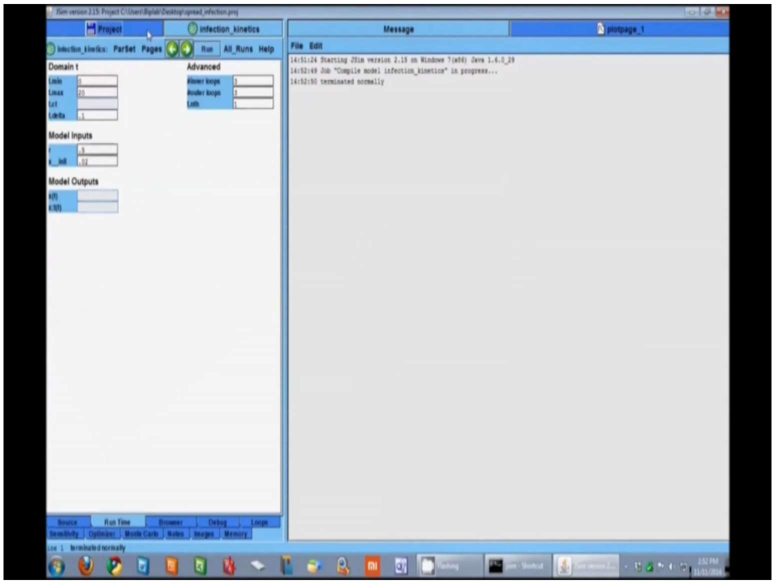
```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
```



```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
```

So we have got the JSim, this is GUI JSim. You can see it has 2 parts, left hand side and right hand side. On left hand side you have options and tools for writing the program and running it. On the right hand side you have the output, either message or the data in plot format. In the file tool if you click you have the options for opening a project. Remember in JSim every work is stored as a project. Inside a project you can have multiple models. You can open an old existing project or you can create a new project. Edit tools give you cut, copy options. Add tools gives you options to import model as I said you can import a SBML model, you can use that. You can create a new model as the option is given. You can add a new data set, you can add a new plot page and all this things. SBW is System Biology Workbench. As an independent tool you can connect to it using this option and you have other preferences and others.

(Refer Slide Time: 10:12)



JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj

Domain t

t.min 0

t.max 20

t.nt

t.delta .1

Model Inputs

r .5

x_init .02

Model Outputs

x(t)

x:t(t)

Advanced

#inner loops 1

#outer loops 1

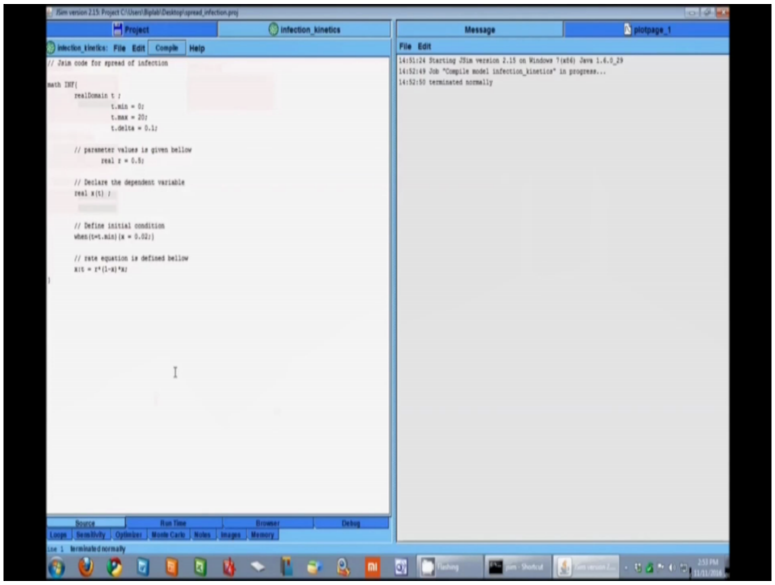
t.sth 1

```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
14:52:49 Job "Compile model infection_kinetics" in progress...
14:52:50 terminated normally
```

Line 1 terminated normally

So let us open an existing project that I have already made. It is in my desktop so I will open it. It is a project to model spread of infectious disease as we have dealt early. Remember all project file have a dot closed extension. So here I have opened that. Notice a new tab has come and this new tab is actually the model as it is shown here infection_kinetic model is the model which simulates the kinetics of spread of infection. So you click on that tab you will get that model. Now see below you have multiple tabs, Tabs for source, runtime and others. Source is the tab where you have the code for this model. Runtime is the tab through which you run the model and you have others like sensitivity optimizer and other else.

(Refer Slide Time: 11:10)

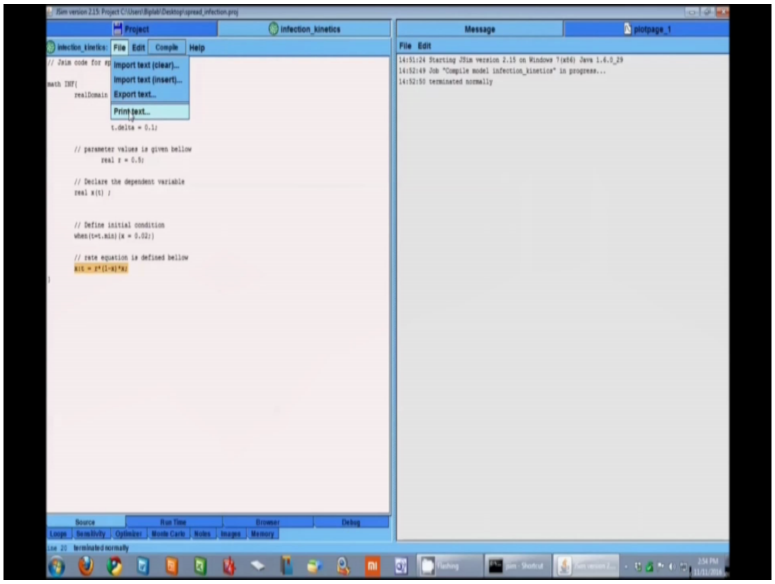

JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
Message
plotpage_1
infection_kinetics: File Edit Compile Help
File Edit
Source
Run Time
Browser
Debug
Loops
Sensitivity
Optimizer
Monte Carlo
Notes
Images
Memory
Line 1 terminated normally

```
// Jsim code for spread of infection

math INF{
        realDomain t ;
                t.min = 0;
                t.max = 20;
                t.delta = 0.1;

        // parameter values is given bellow
              real r = 0.5;

        // Declare the dependent variable
        real x(t) ;


        // Define initial condition
        when(t=t.min)(x = 0.02;)

        // rate equation is defined bellow
        x:t = r*(1-x)*x;
}
```

```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
14:52:49 Job "Compile model infection_kinetics" in progress...
14:52:50 terminated normally
```

Let us see the source. This is the code for the model of spread of infectious disease. I will discuss how to write this code later on. Let us just look into it, you may recognize one equation that (R*1) – (x*x) that is there which represents spread of infection. So this is the ordinary differential equation written in JSIM code to model the spread of infectious disease.

(Refer Slide Time: 11:48)

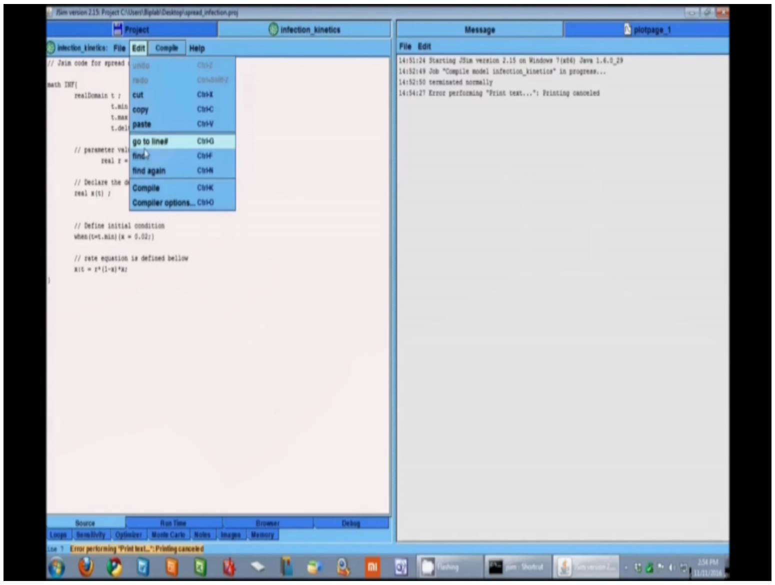


```
// Jsim code for sp

math INF{
        realDomain

                t.delta = 0.1;

        // parameter values is given bellow
              real r = 0.5;

        // Declare the dependent variable
        real x(t) ;


        // Define initial condition
        when(t=t.min)(x = 0.02;)

        // rate equation is defined bellow
        x:t = r*(1-x)*x;
}
```

```
14:51:24
14:52:49
14:52:50
```

In this page you have multiple options like file. I can print this code by print text option. So you can print it. We will not do it here.

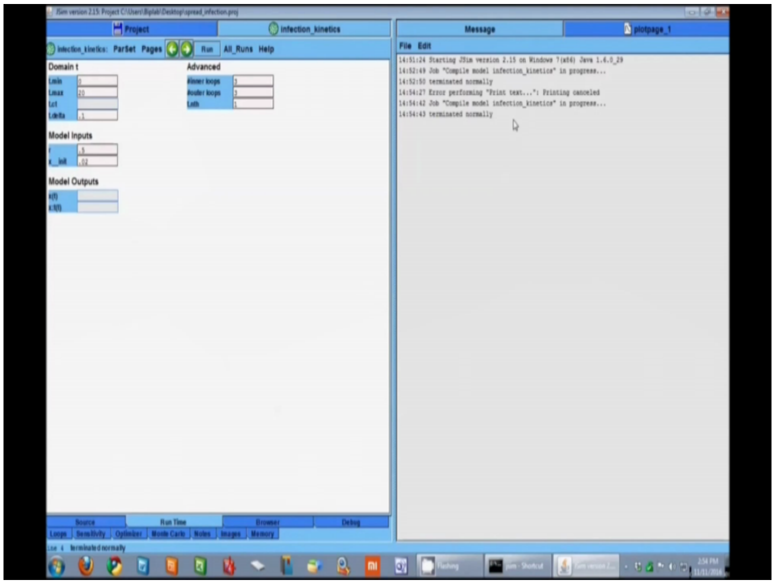
(Refer Slide Time: 12:00)


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
Message
plotpage_1
infection_kinetics: File Edit Compile Help
undo Ctrl-Z
redo Ctrl-Shift-Z
cut Ctrl-X
copy Ctrl-C
paste Ctrl-V
go to line# Ctrl-G
find... Ctrl-F
find again Ctrl-N
Compile Ctrl-K
Compiler options... Ctrl-O
File Edit
Source Run Time Browser Debug
Loops Sensitivity Optimizer Monte Carlo Notes Images Memory

```
// Jsim code for spread
math INF{
        realDomain t ;
                t.min
                t.max
                t.del

        // parameter val
                real r =

        // Declare the d
        real x(t) ;

        // Define initial condition
        when(t=t.min)(x = 0.02;)

        // rate equation is defined bellow
        x:t = r*(1-x)*x;
}
```

```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
14:52:49 Job "Compile model infection_kinetics" in progress...
14:52:50 terminated normally
14:54:27 Error performing "Print text...": Printing canceled
```

Line 7 Error performing "Print text...": Printing canceled


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
Message
plotpage_1
infection_kinetics: ParSet Pages Run All_Runs Help
File Edit
Source Run Time Browser Debug
Loops Sensitivity Optimizer Monte Carlo Notes Images Memory

Domain t

t.min 0

t.max 20

t.ct

t.delta .1

Advanced

#inner loops 1

#outer loops 1

t.eth 1

Model Inputs

r .5

x_init .02

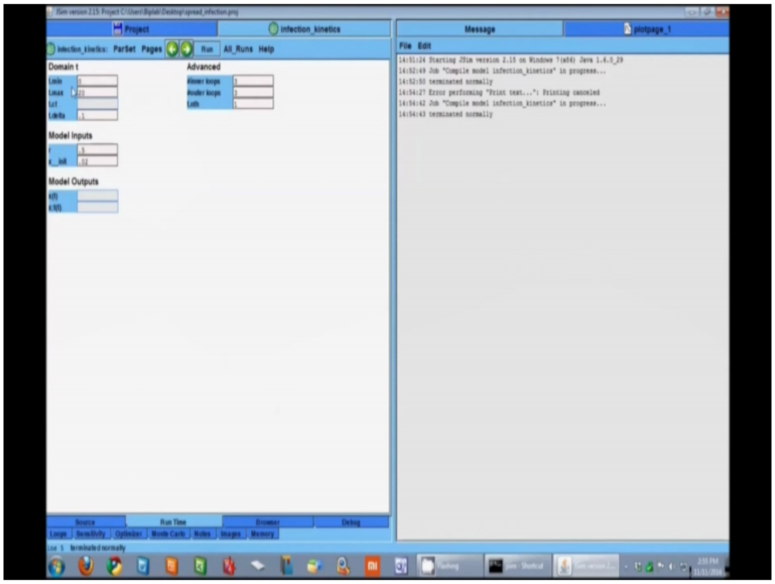
Model Outputs

x(t)

x:t(t)

```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
14:52:49 Job "Compile model infection_kinetics" in progress...
14:52:50 terminated normally
14:54:27 Error performing "Print text...": Printing canceled
14:54:42 Job "Compile model infection_kinetics" in progress...
14:54:43 terminated normally
```

Line 4 terminated normally


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
Message
plotpage_1
infection_kinetics: ParSet Pages Run All_Runs Help
File Edit
Source
Run Time
Browser
Debug
Loops Sensitivity Optimizer Monte Carlo Notes Images Memory

Domain t

t.min 0
t.max 20
t.ct
t.delta .1

Advanced

#inner loops 1
#outer loops 1
t.nth 1

Model Inputs

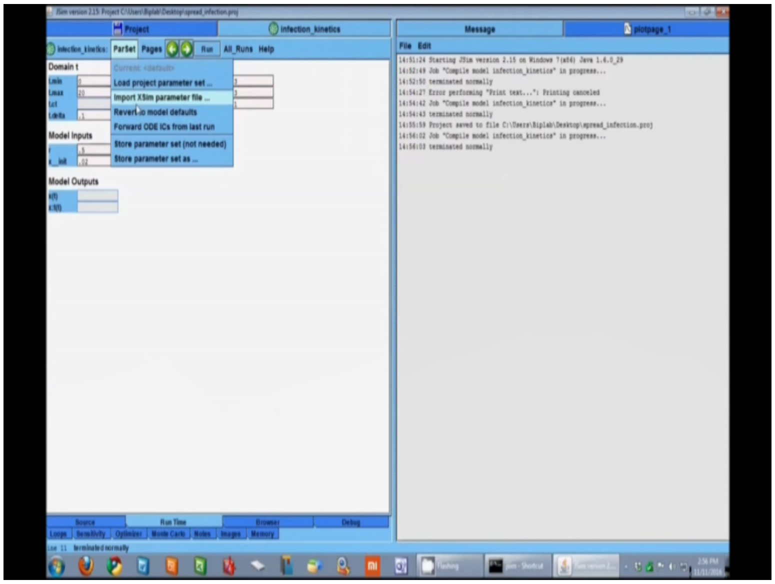
r .5
x_init .02

Model Outputs

x(t)
x:t(t)

```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
14:52:49 Job "Compile model infection_kinetics" in progress...
14:52:50 terminated normally
14:54:27 Error performing "Print text...": Printing canceled
14:54:42 Job "Compile model infection_kinetics" in progress...
14:54:43 terminated normally
```

Line 5 terminated normally


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
Message
plotpage_1
infection_kinetics: ParSet Pages Run All_Runs Help
Current: <default>
Load project parameter set ...
Import XSim parameter file ...
Revert to model defaults
Forward ODE ICs from last run
Store parameter set (not needed)
Store parameter set as ...
File Edit
Source
Run Time
Browser
Debug
Loops Sensitivity Optimizer Monte Carlo Notes Images Memory

Domain t

t.min 0
t.max 20
t.ct
t.delta .1

Model Inputs

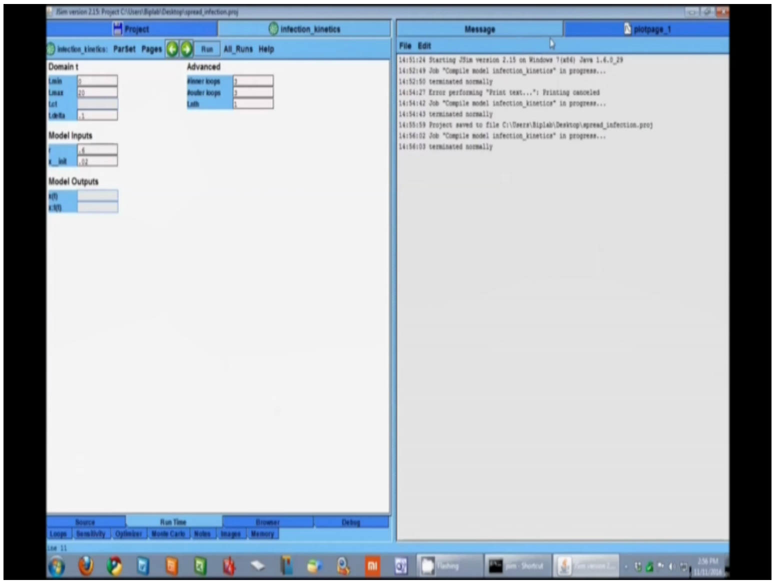
r .5
x_init .02

Model Outputs

x(t)
x:t(t)

```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
14:52:49 Job "Compile model infection_kinetics" in progress...
14:52:50 terminated normally
14:54:27 Error performing "Print text...": Printing canceled
14:54:42 Job "Compile model infection_kinetics" in progress...
14:54:43 terminated normally
14:55:59 Project saved to file C:\Users\Biplab\Desktop\spread_infection.proj
14:56:02 Job "Compile model infection_kinetics" in progress...
14:56:03 terminated normally
```

Line 11 terminated normally


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
infection_kinetics: ParSet Pages Run All_Runs Help
Message
plotpage_1
File Edit
Source
Run Time
Browser
Debug

Domain t

t.min	0
t.max	20
t.ct	
t.delta	.1

Advanced

#inner loops	1
#outer loops	3
t.sth	1

Model Inputs

r	.6
x__init	.02

Model Outputs

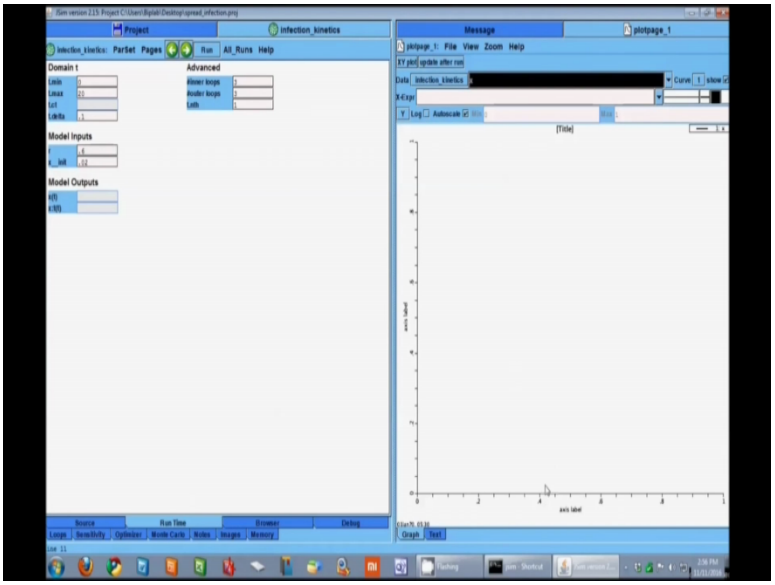
x(t)	
x:t(t)	

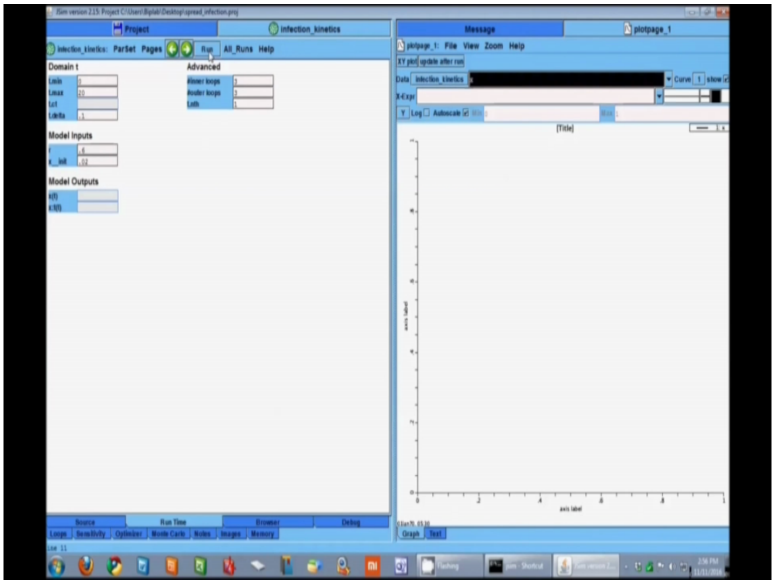
```
14:51:24 Starting JSim version 2.15 on Windows 7(x86) Java 1.6.0_29
14:52:49 Job "Compile model infection_kinetics" in progress...
14:52:50 terminated normally
14:54:27 Error performing "Print text...": Printing canceled
14:54:42 Job "Compile model infection_kinetics" in progress...
14:54:43 terminated normally
14:55:59 Project saved to file C:\Users\Biplab\Desktop\spread_infection.proj
14:56:02 Job "Compile model infection_kinetics" in progress...
14:56:03 terminated normally
```

You have edit option by which you can copy, paste the code or you can find the code plot and notice that there is a button compile, once you have written down the code you have to compile it so that JSim can run it. Once you compile successfully this runtime tab gets activated and you reach this runtime tab. You can see the message even though it is written that chopped compile model infection kinetic in progress terminated normal. That means JSim has successfully compiled the program. In the runtime tab you have multiple information. Each of these values are values of variables which I can change for example T min is 0.

There is a minimum time of and this is coming from the code block here T min = 0. So either you change in the code or you go to the runtime window and change these values. I can change the value of T max. T max I have said is 20, I can change it. I can change the value of R, x initial. There is an initial value of x. All these things I can change either in the source code or in the runtime window. So I have changed that, I have saved it and I will go back and compile again. Now I have change from parameter set revert to model default so that the value changed in the code get executed. So in model input R has changed from 0.5 to 0.6.

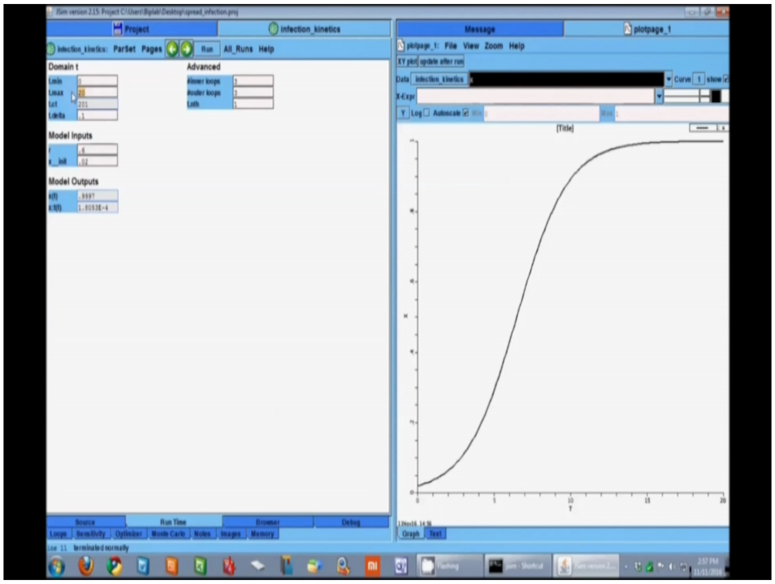
(Refer Slide Time: 14:05)





Now we are going to run and see the output in the plot page. In the plot page you select the model. We have only one model. You select a variable i.e. x is the only variable so you selected it. Now horizontal axis is the time and vertical axis is for the dependent variable x. Let us run it clicking run. You got the result. You can see the typical sigmoidal curve. Change the name of the axis. Vertical axis is x and horizontal axis is time T. So now we have the data.

(Refer Slide Time: 14:43)


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
Message
plotpage_1
infection_kinetics: ParSet Pages Run All_Runs Help
plotpage_1: File View Zoom Help
[Title]
Source
Run Time
Browser
Debug
Graph
Text

Domain t
t.min 0
t.max 20
t.ct 201
t.delta .1

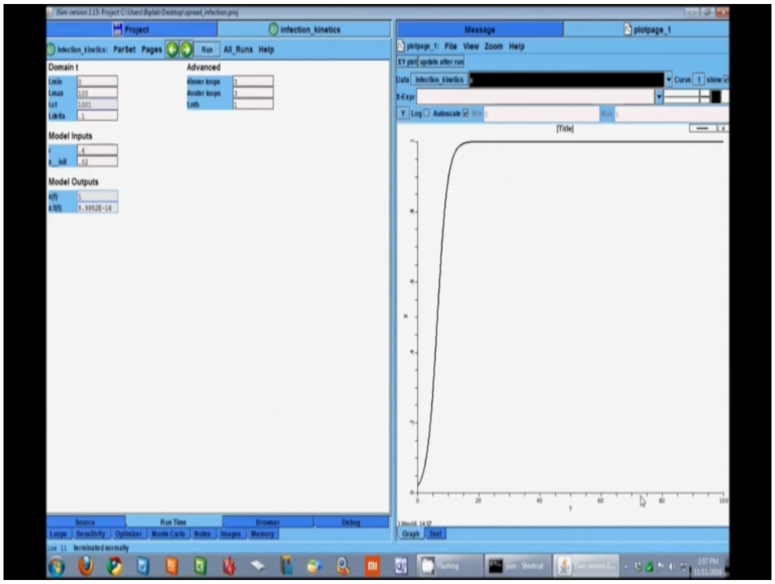
Advanced
#inner loops 1
#outer loops 3
t.nth 1

Model Inputs
r .6
x__init .02

Model Outputs
x(t) .9997
x:t(t) 1.8053E-4

I can now change the total time of simulation from 20 to 100. Now run again. Notice the horizontal axis; it has changed up to 100.

(Refer Slide Time: 14:56)


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
Message
plotpage_1
infection_kinetics: ParSet Pages Run All_Runs Help
plotpage_1: File View Zoom Help
[Title]
0
20
40
60
80
100
Source
Run Time
Browser
Debug
Graph
Text

Domain t
t.min 0
t.max 100
t.ct 1001
t.delta .1

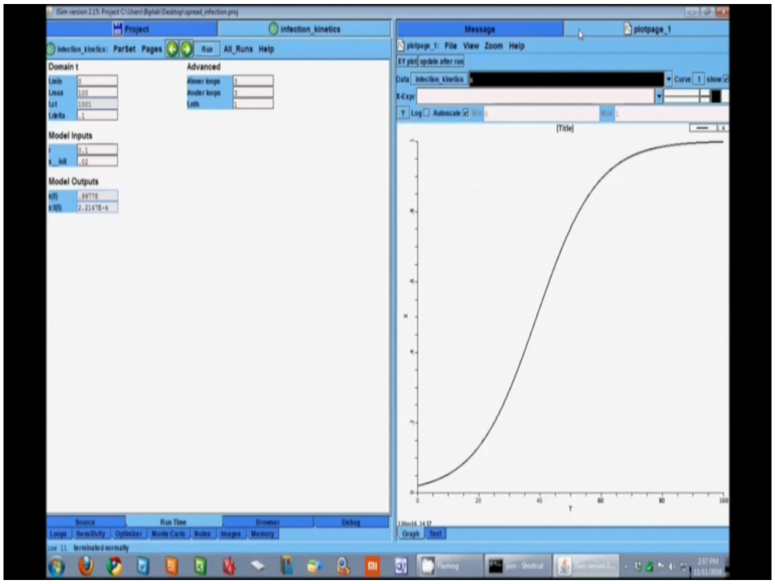
Advanced
#inner loops 1
#outer loops 3
t.nth 1

Model Inputs
r .6
x__init .02

Model Outputs
x(t) 1
x:t(t) 5.9952E-14

Now let us change the model input R, the rate constant to 0.1, run again. You see the pattern of change of x with respect to time has changed.

(Refer Slide Time: 15:09)



Domain t

t.min	0
t.max	100
t.ct	1001
t.delta	.1

Advanced

#inner loops	1
#outer loops	1
t.nth	1

Model Inputs

r	0.1
x__init	.02

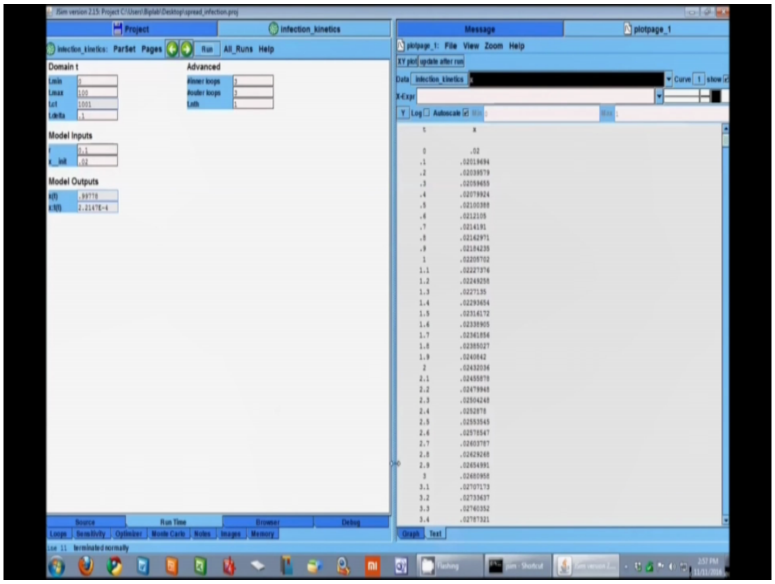
Model Outputs

x(t)	.99778
x:t(t)	2.2147E-4

Data infection_kinetics x

Y Log □ Autoscale ☑

Line 11 terminated normally



Domain t

t.min	0
t.max	100
t.ct	1001
t.delta	.1

Advanced

#inner loops	1
#outer loops	1
t.nth	1

Model Inputs

r	0.1
x__init	.02

Model Outputs

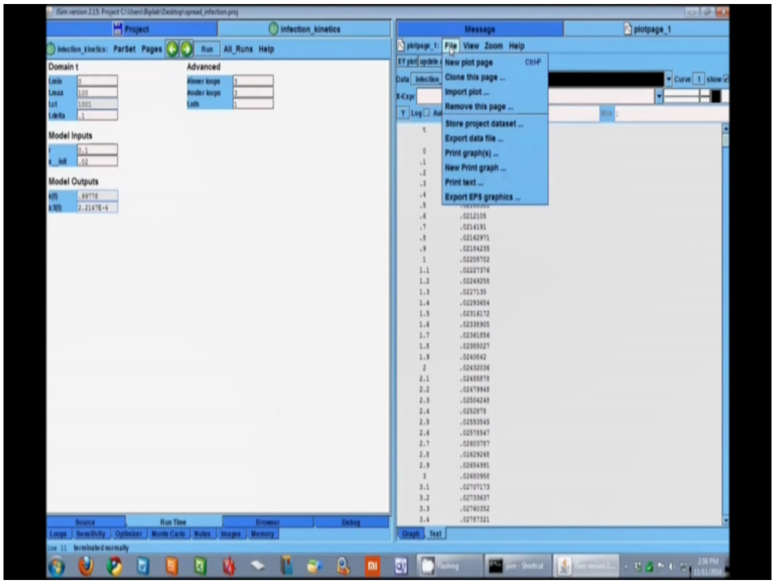
x(t)	.99778
x:t(t)	2.2147E-4

Data infection_kinetics x

Y Log □ Autoscale ☑

```
     t          x

     0         .02
    .1    .02019694
    .2    .02039579
    .3    .02059655
    .4    .02079924
    .5    .02100388
    .6    .0212105
    .7    .0214191
    .8    .02162971
    .9    .02184235
     1    .02205702
   1.1    .02227376
   1.2    .02249258
   1.3    .0227135
   1.4    .02293654
   1.5    .02316172
   1.6    .02338905
   1.7    .02361856
   1.8    .02385027
   1.9    .0240842
     2    .02432036
   2.1    .02455878
   2.2    .02479948
   2.3    .02504248
   2.4    .0252878
   2.5    .02553545
   2.6    .02578547
   2.7    .02603787
   2.8    .02629268
   2.9    .02654991
     3    .02680958
   3.1    .02707173
   3.2    .02733637
   3.3    .02760352
   3.4    .02787321
```

Line 11 terminated normally



Domain t

t.min	0
t.max	100
t.ct	1001
t.delta	.1

Advanced

#inner loops	1
#outer loops	3
t.nth	1

Model Inputs

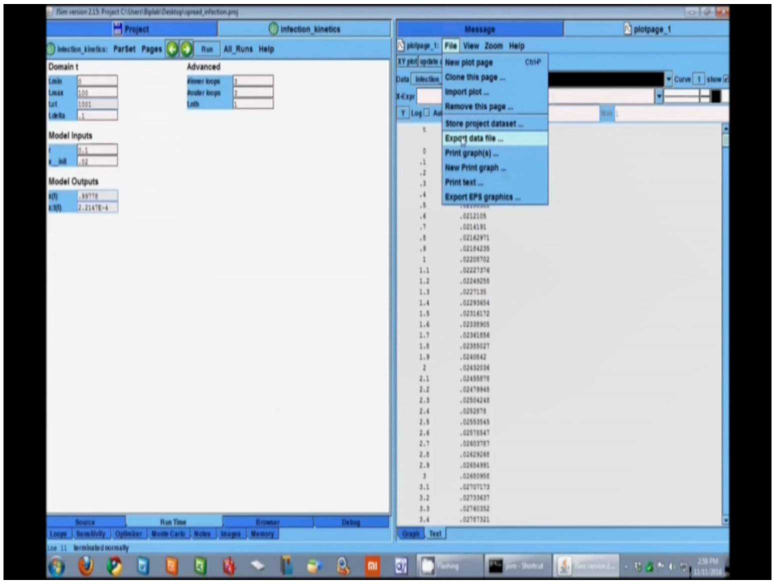
r	0.1
x__init	.02

Model Outputs

x(t)	.99778
x:t(t)	2.2147E-4

```
  t

  0
 .1
 .2
 .3
 .4
 .5
 .6        .0212105
 .7        .0214191
 .8        .02162971
 .9        .02184235
  1        .02205702
1.1        .02227376
1.2        .02249258
1.3        .0227135
1.4        .02293654
1.5        .02316172
1.6        .02338905
1.7        .02361856
1.8        .02385027
1.9        .0240842
  2        .02432036
2.1        .02455878
2.2        .02479948
2.3        .02504248
2.4        .0252878
2.5        .02553545
2.6        .02578547
2.7        .02603787
2.8        .02629268
2.9        .02654991
  3        .02680958
3.1        .02707173
3.2        .02733637
3.3        .02760352
3.4        .02787321
```

Line 11 terminated normally


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj

Domain t

t.min	0
t.max	100
t.ct	1001
t.delta	.1

Advanced

#inner loops	1
#outer loops	3
t.nth	1

Model Inputs

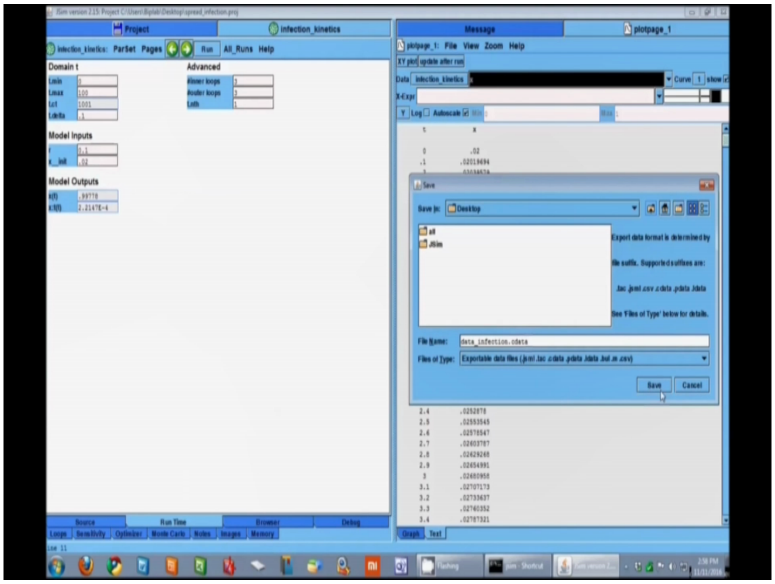
r	0.1
x__init	.02

Model Outputs

x(t)	.99778
x:t(t)	2.2147E-4

```
  t

  0
 .1
 .2
 .3
 .4
 .5
 .6        .0212105
 .7        .0214191
 .8        .02162971
 .9        .02184235
  1        .02205702
1.1        .02227376
1.2        .02249258
1.3        .0227135
1.4        .02293654
1.5        .02316172
1.6        .02338905
1.7        .02361856
1.8        .02385027
1.9        .0240842
  2        .02432036
2.1        .02455878
2.2        .02479948
2.3        .02504248
2.4        .0252878
2.5        .02553545
2.6        .02578547
2.7        .02603787
2.8        .02629268
2.9        .02654991
  3        .02680958
3.1        .02707173
3.2        .02733637
3.3        .02760352
3.4        .02787321
```

Line 11 terminated normally



JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj

Domain t
tmin 0
tmax 100
tct 1001
tdelta .1

Advanced
#inner loops 1
#outer loops 1
tsfh 1

Model Inputs
r 0.1
x_init .02

Model Outputs
x(t) .99778
x:t(t) 2.2147E-4

Save in: Desktop

Export data format is determined by file suffix. Supported suffixes are: .tac .jsml .csv .cdata .pdata .ldata See 'Files of Type' below for details.

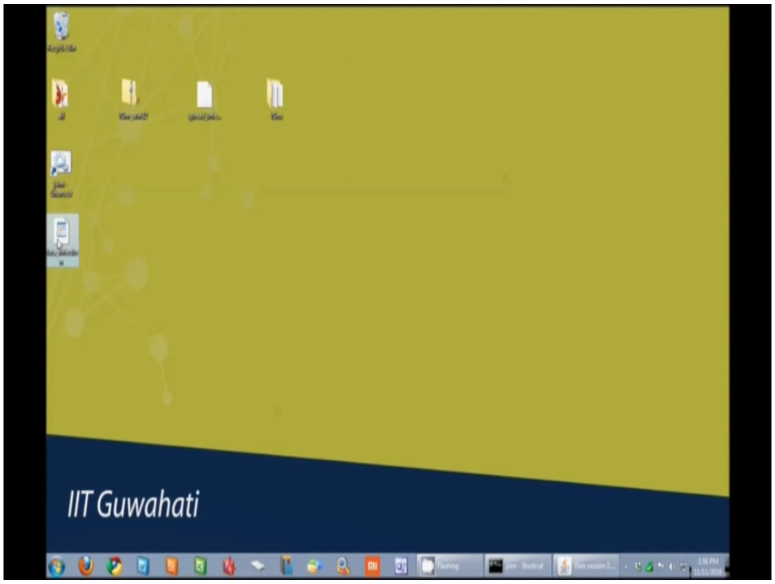
File Name: data_infection.cdata

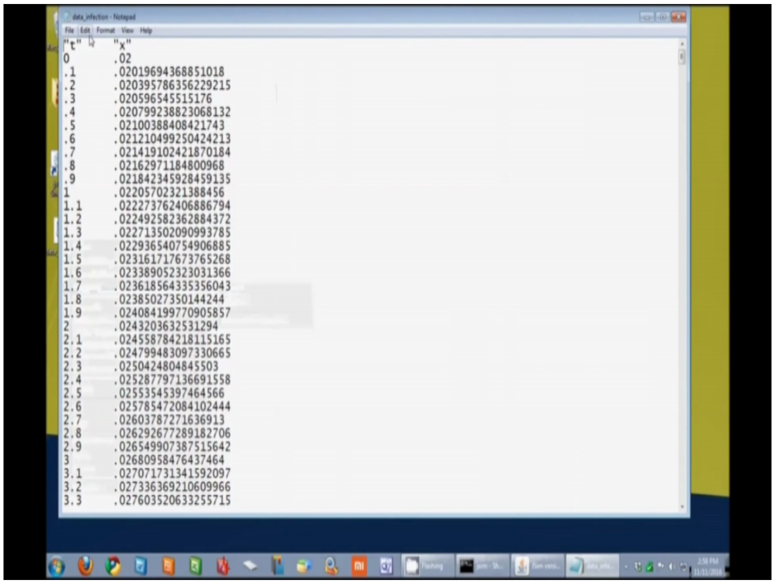
Files of Type: Exportable data files (.jsml .tac .cdata .pdata .ldata .bsl .m .csv)

```
t       x
0       .02
.1      .02019694
2.4     .0252878
2.5     .02553545
2.6     .02578547
2.7     .02603787
2.8     .02629268
2.9     .02654991
3       .02680958
3.1     .02707173
3.2     .02733637
3.3     .02760352
3.4     .02787321
```

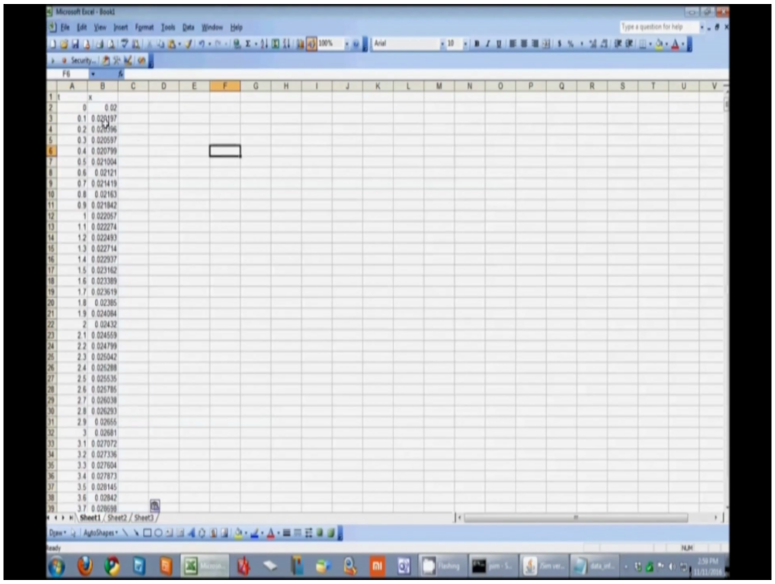
Apart from this visualization JSIM also gives you the data in text format as shown in this tab. It is a separate tab named as text. Interestingly I can save this data as a text file so that that text file can be opened in another software and analyzed. So go to file. There you have option of export data file. JSIM allow you to export data in different format from comma separated to tab delimited. I will save this data in C data format, give a name and then put the extension. Don't forget to put the extension in the file name. I will use C data as a extension. So name of my file is Data_infection.cdata, save it. Once you save, the data has got as a text file.

(Refer Slide Time: 16:26)

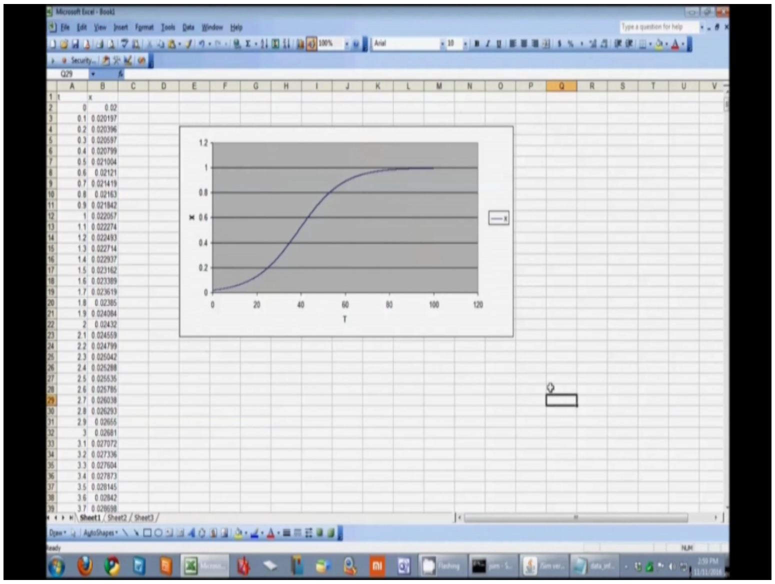




```
"t"     "x"
0       .02
.1      .020196943688510l8
.2      .0203957863562292l5
.3      .020596545515176
.4      .020799238823068132
.5      .021003884084217 43
.6      .021210499250424213
.7      .021419102421870184
.8      .0216297118480096 8
.9      .021842345928459135
1       .0220570232138845 6
1.1     .022273762406886794
1.2     .022492582362884372
1.3     .022713502090993785
1.4     .022936540754906885
1.5     .023161717673765268
1.6     .023389052323031366
1.7     .023618564335356043
1.8     .0238502735014424 4
1.9     .024084199770905857
2       .024320363253129 4
2.1     .024558784218115165
2.2     .024799483097330665
2.3     .025042480484550 3
2.4     .025287797136691558
2.5     .0255354539746456 6
2.6     .025785472084102444
2.7     .0260378727163691 3
2.8     .026292677289182706
2.9     .026549907387515642
3       .0268095847643746 4
3.1     .027071731341592097
3.2     .027336369210609966
3.3     .027603520633255715
```



	A	B
1	t	x
2	0	0.02
3	0.1	0.020197
4	0.2	0.020396
5	0.3	0.020597
6	0.4	0.020799
7	0.5	0.021004
8	0.6	0.02121
9	0.7	0.021419
10	0.8	0.02163
11	0.9	0.021842
12	1	0.022057
13	1.1	0.022274
14	1.2	0.022493
15	1.3	0.022714
16	1.4	0.022937
17	1.5	0.023162
18	1.6	0.023389
19	1.7	0.023619
20	1.8	0.02385
21	1.9	0.024084
22	2	0.02432
23	2.1	0.024559
24	2.2	0.024799
25	2.3	0.025042
26	2.4	0.025288
27	2.5	0.025535
28	2.6	0.025785
29	2.7	0.026038
30	2.8	0.026293
31	2.9	0.02655
32	3	0.02681
33	3.1	0.027072
34	3.2	0.027336
35	3.3	0.027604
36	3.4	0.027873
37	3.5	0.028145
38	3.6	0.02842
39	3.7	0.028698

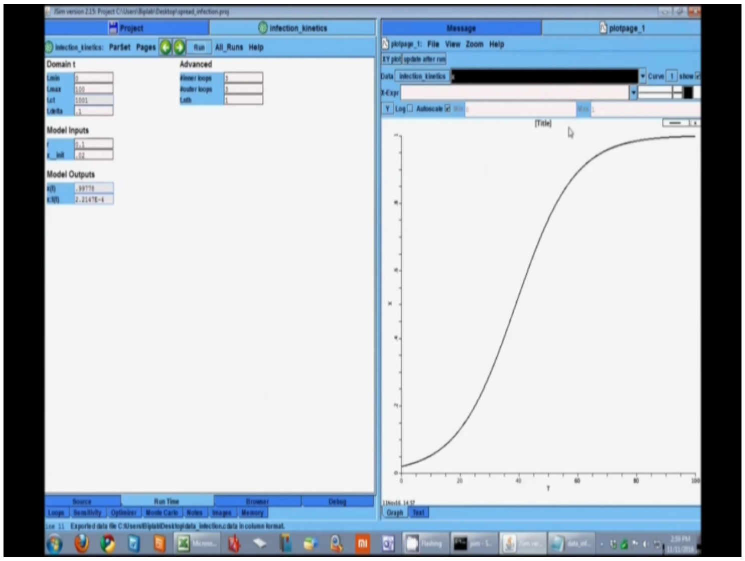


Microsoft Excel - Book1

	A	B
1	t	x
2	0	0.02
3	0.1	0.020197
4	0.2	0.020396
5	0.3	0.020597
6	0.4	0.020799
7	0.5	0.021004
8	0.6	0.02121
9	0.7	0.021419
10	0.8	0.02163
11	0.9	0.021842
12	1	0.022057
13	1.1	0.022274
14	1.2	0.022493
15	1.3	0.022714
16	1.4	0.022937
17	1.5	0.023162
18	1.6	0.023389
19	1.7	0.023619
20	1.8	0.02385
21	1.9	0.024084
22	2	0.02432
23	2.1	0.024559
24	2.2	0.024799
25	2.3	0.025042
26	2.4	0.025288
27	2.5	0.025535
28	2.6	0.025785
29	2.7	0.026038
30	2.8	0.026293
31	2.9	0.02655
32	3	0.02681
33	3.1	0.027072
34	3.2	0.027336
35	3.3	0.027604
36	3.4	0.027873
37	3.5	0.028145
38	3.6	0.02842
39	3.7	0.028698

Let us see that. Here I have the text file. I can open it in a notepad or WordPad. I can simply select all data and copy and paste it into some other software like Microsoft excel. Let's open a Microsoft excel page, paste it here. So now I have exported the data and I have it in Microsoft excel. So I can use the graphic tool of Microsoft excel to draw the graph here and do all the manipulation and formatting which are not possible in JSIM. For example if you want to change font size or color or put some background text or put some background color, JSIM will not allow you to do that you can do that here in Microsoft excel. So here we go we have the same graph.

(Refer Slide Time: 17:24)



JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj

Domain t

t.min	0
t.max	100
t.ct	1001
t.delta	.1

Advanced

#inner loops	1
#outer loops	1
t.nth	1

Model Inputs

r	0.1
x_init	.02

Model Outputs

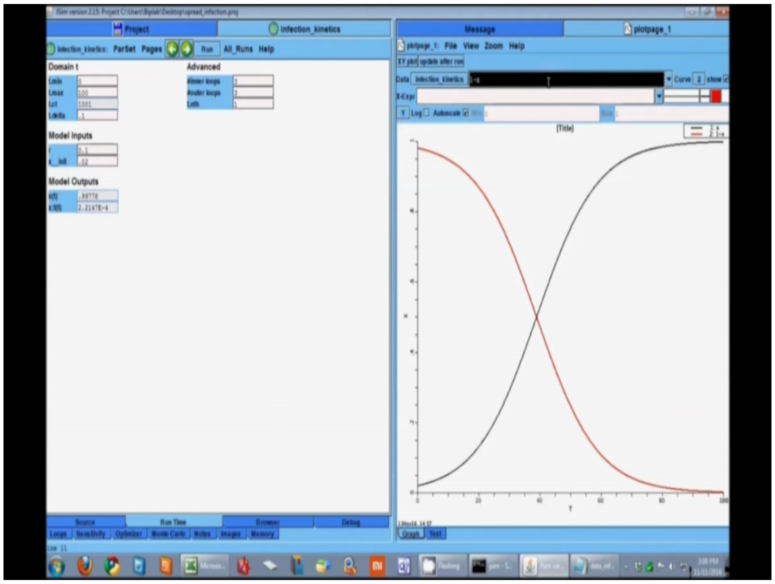
x(t)	.99778
x:t(t)	2.2147E-4

Data infection_kinetics x Curve 1 show ☑

Y Log □ Autoscale ☑ Min 0 Max 1

Line 11 Exported data file C:\Users\Biplab\Desktop\data_infection.cdata in column format.

Project
infection_kinetics
infection_kinetics: ParSet Pages Run All_Runs Help
Message
plotpage_1
plotpage_1: File View Zoom Help
XY plot update after run
X-Expr
[Title]
x
0
20
40
60
80
100
T
11Nov16, 14:57
Graph Text
Source Run Time Browser Debug
Loops Sensitivity Optimizer Monte Carlo Notes Images Memory



JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj

Domain t

t.min	0
t.max	100
t.ct	1001
t.delta	.1

Advanced

#inner loops	1
#outer loops	1
t.nth	1

Model Inputs

r	0.1
x__init	.02

Model Outputs

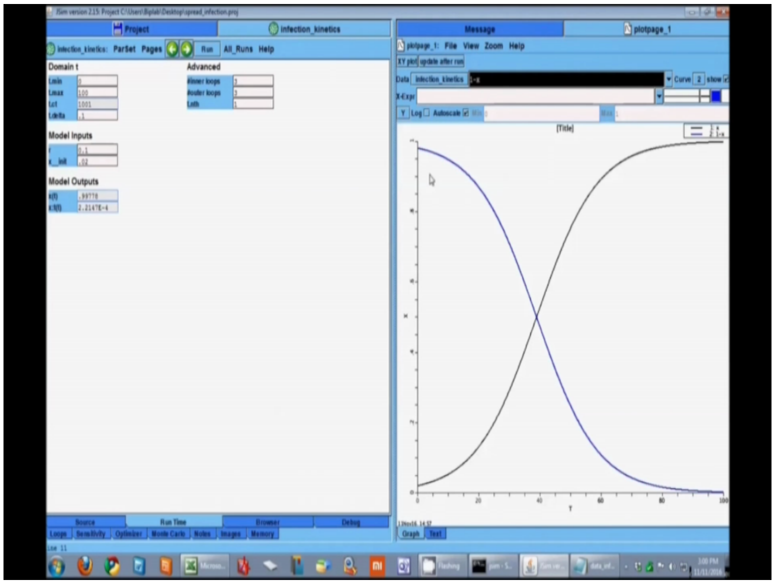
x(t)	.99778
x:t(t)	2.2147E-4

Data infection_kinetics 1-x Curve 2 show ☑

X-Expr

Y Log □ Autoscale ☑ Min 0 Max 1

Project
infection_kinetics
infection_kinetics: ParSet Pages Run All_Runs Help
Message
plotpage_1
plotpage_1: File View Zoom Help
XY plot update after run
[Title]
1 x
2 1-x
0
20
40
60
80
100
Source
Run Time
Browser
Debug
Loops Sensitivity Optimizer Monte Carlo Notes Images Memory
Graph Text



JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj

Domain t

t.min	0
t.max	100
t.ct	1001
t.delta	.1

Advanced

#inner loops	1
#outer loops	1
t.nth	1

Model Inputs

r	0.1
x__init	.02

Model Outputs

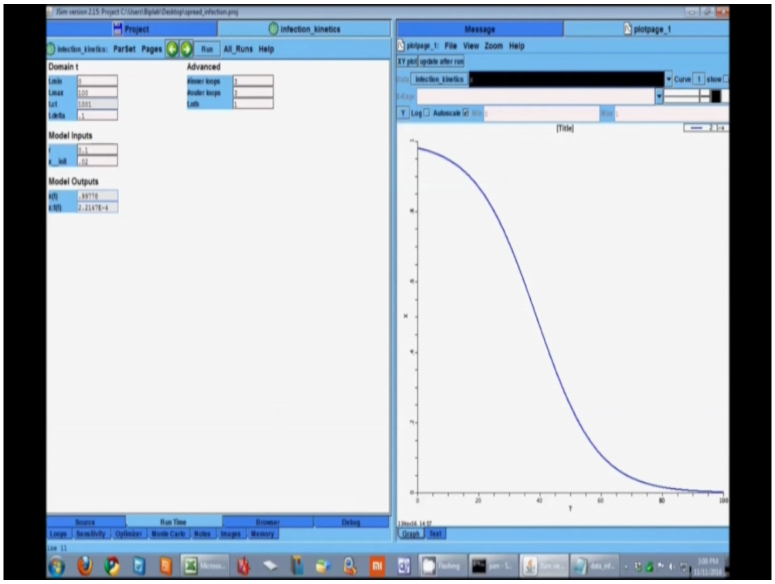
x(t)	.99778
x:t(t)	2.2147E-4

Data infection_kinetics 1-x Curve 2 show ☑

X-Expr

Y Log □ Autoscale ☑ Min 0 Max 1

Project
infection_kinetics
infection_kinetics: ParSet Pages Run All_Runs Help
Message
plotpage_1
plotpage_1: File View Zoom Help
XY plot update after run
[Title]
1 x
2 1-x
0
20
40
60
80
100
Source
Run Time
Browser
Debug
Loops Sensitivity Optimizer Monte Carlo Notes Images Memory
Graph Text


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
Message
plotpage_1
infection_kinetics: ParSet Pages Run All_Runs Help
plotpage_1: File View Zoom Help
XY plot update after run
Data infection_kinetics
Curve 1 show
X-Expr
Y Log Autoscale
[Title]
Source Run Time Browser Debug
Loops Sensitivity Optimizer Monte Carlo Notes Images Memory
Graph Text

Domain t

t.min	0
t.max	100
t.ct	1001
t.delta	.1

Advanced

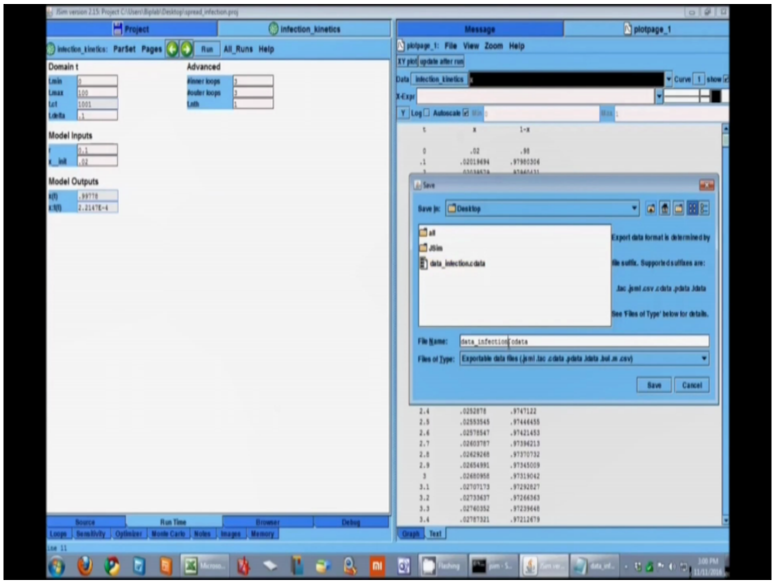
#inner loops	1
#outer loops	3
t.nth	1

Model Inputs

r	0.1
x__init	.02

Model Outputs

x(t)	.99778
x:t(t)	2.2147E-4


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
Message
plotpage_1
infection_kinetics: ParSet Pages Run All_Runs Help
plotpage_1: File View Zoom Help
XY plot update after run
Data infection_kinetics
Curve 1 show
X-Expr
Y Log Autoscale
Save
Save Cancel
Source Run Time Browser Debug
Loops Sensitivity Optimizer Monte Carlo Notes Images Memory
Graph Text

Save in: Desktop

all
JSim
data_infection.cdata

Export data format is determined by file suffix. Supported suffixes are: .tac .jsml .csv .cdata .pdata .ldata See 'Files of Type' below for details.

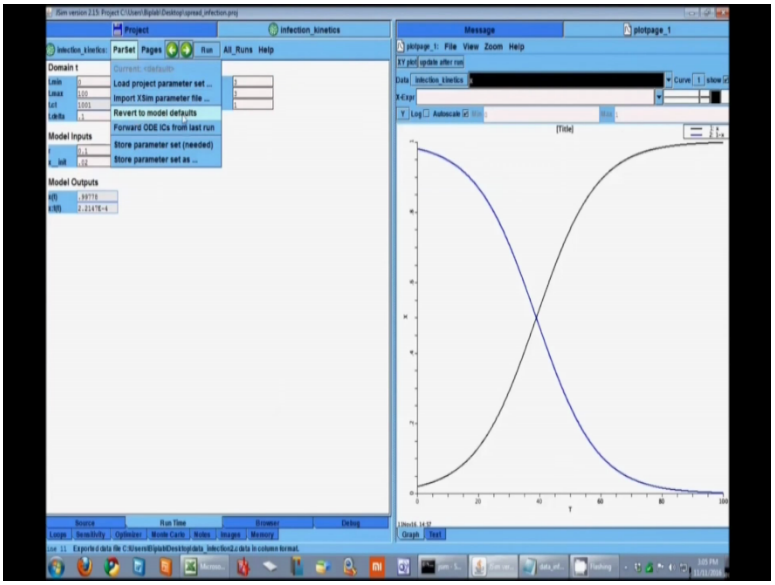
File Name: data_infection.cdata

Files of Type: Exportable data files (.jsml .tac .cdata .pdata .ldata .bol .m .csv)

```
  t         x           1-x

  0        .02          .98
 .1     .02019694    .97980306
2.4     .0252878     .9747122
2.5     .02553545    .97446455
2.6     .02578547    .97421453
2.7     .02603787    .97396213
2.8     .02629268    .97370732
2.9     .02654991    .97345009
 3      .02680958    .97319042
3.1     .02707173    .97292827
3.2     .02733637    .97266363
3.3     .02760352    .97239648
3.4     .02787321    .97212679
```

So we have the graph here and that data is depending upon specific value of the input parameter. We can put multi if we have a model with multiple parameters. We can draw them here also by choosing multiple curves. For example suppose I want to plot (1-x) so I updated a new curve and defined it as (1-x) and changed, put the color blue in that. If I want to remove it I can simply uncheck the show option. I can go to 1 and uncheck that so x will disappear. So in this way multiple variables you can show and check uncheck and change their color depending upon your utility. So as you show in the graph, your data will be shown in the text format also. You can also export that data. I will save it as 2nd file and remember the extension was cdata.

(Refer Slide Time: 18:41)


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
infection_kinetics: ParSet Pages Run All_Runs Help
Current: <default>
Load project parameter set ...
Import XSim parameter file ...
Revert to model defaults
Forward ODE ICs from last run
Store parameter set (needed)
Store parameter set as ...
Message
plotpage_1
[Title]

Domain t

t.min	0
t.max	100
t.ct	1001
t.delta	.1

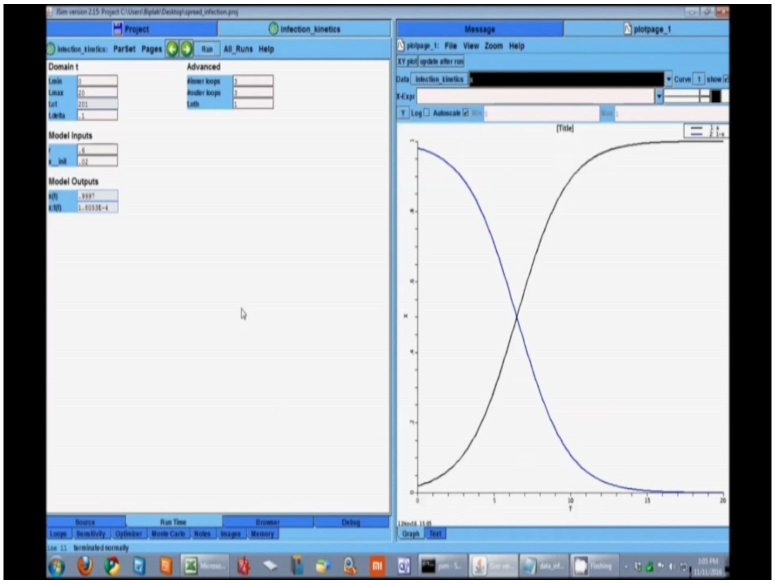
Model Inputs

r	0.1
x__init	.02

Model Outputs

x(t)	.99778
x:t(t)	2.2147E-4

Exported data file C:\Users\Biplab\Desktop\data_infection2.z.data in column format.


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
infection_kinetics: ParSet Pages Run All_Runs Help
Message
plotpage_1
[Title]

Domain t

t.min	0
t.max	20
t.ct	201
t.delta	.1

Advanced

#inner loops	3
#outer loops	3
t.nth	1

Model Inputs

r	.6
x__init	.02

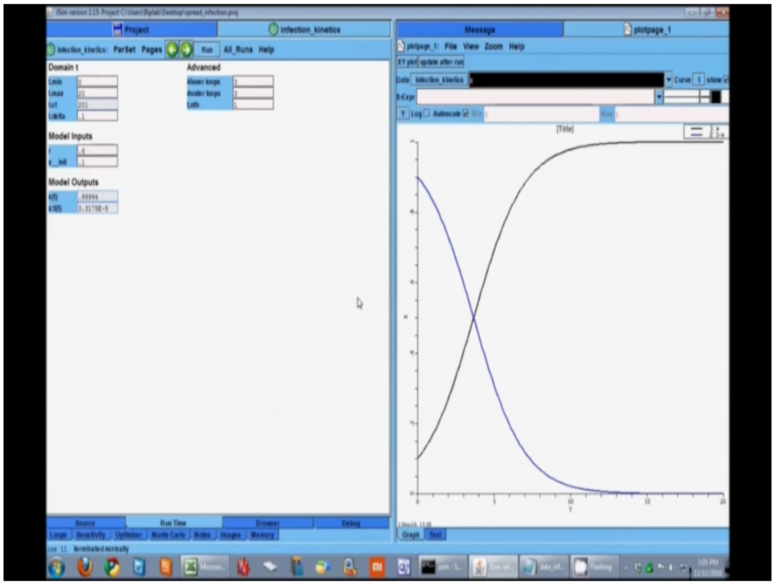
Model Outputs

x(t)	.9997
x:t(t)	1.8053E-4

terminated normally

Now in this module we have used r = 0.1. We can revert back to the model default. The default value of the parameters will become 0.6 because in the code I have written that as 0.6. Let us run once again.

(Refer Slide Time: 19:10)


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
infection_kinetics: ParSet Pages Run All_Runs Help
Message
plotpage_1
plotpage_1: File View Zoom Help
[Title]

Domain t
tmin 0
tmax 20
t.ct 201
t.delta .1

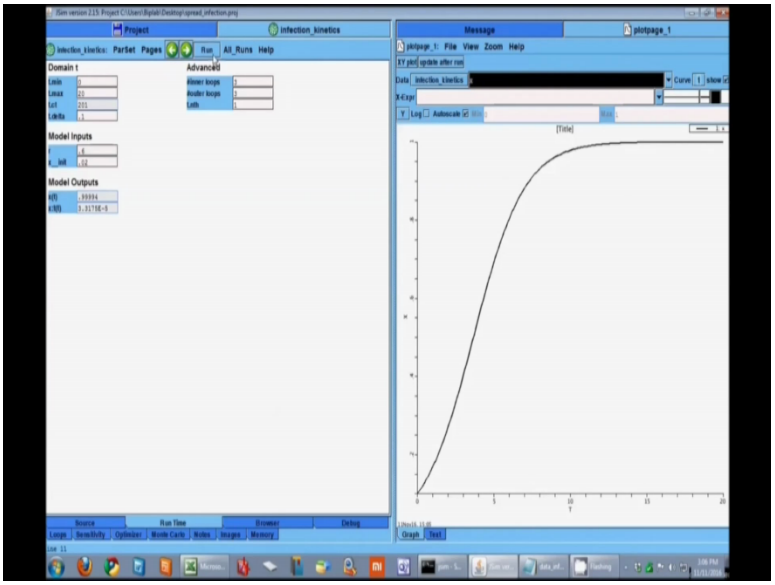
Advanced
#inner loops 3
#outer loops 3
t.nth 1

Model Inputs
r .6
x_init .1

Model Outputs
x(t) .99994
x:t(t) 3.3175E-5

Now let us change the initial value of x and run it again. So you see how the graph has changed. So the x is now starting from 0.1 and we have corresponding (1-x) plot also. Let us go back again to the original value of 0.02.

(Refer Slide Time: 19:34)


JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj
Project
infection_kinetics
infection_kinetics: ParSet Pages Run All_Runs Help
Message
plotpage_1
plotpage_1: File View Zoom Help
[Title]

Domain t
tmin 0
tmax 20
t.ct 201
t.delta .1

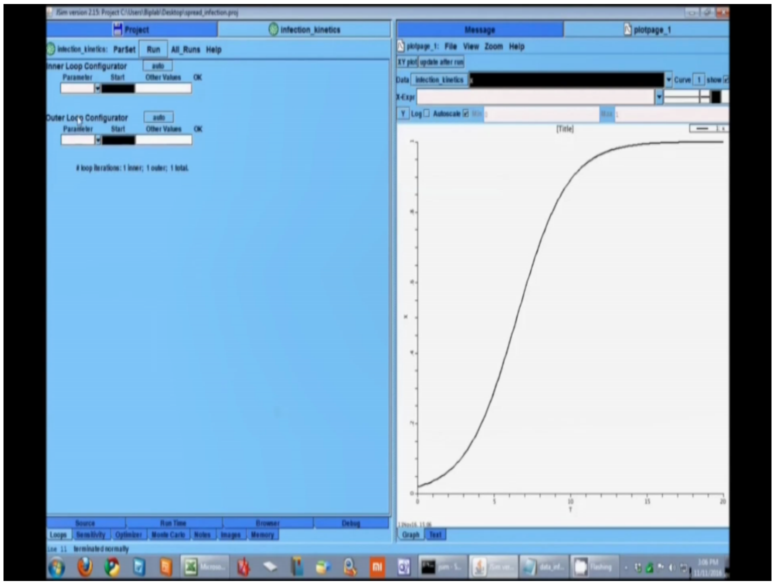
Advanced
#inner loops 3
#outer loops 3
t.nth 1

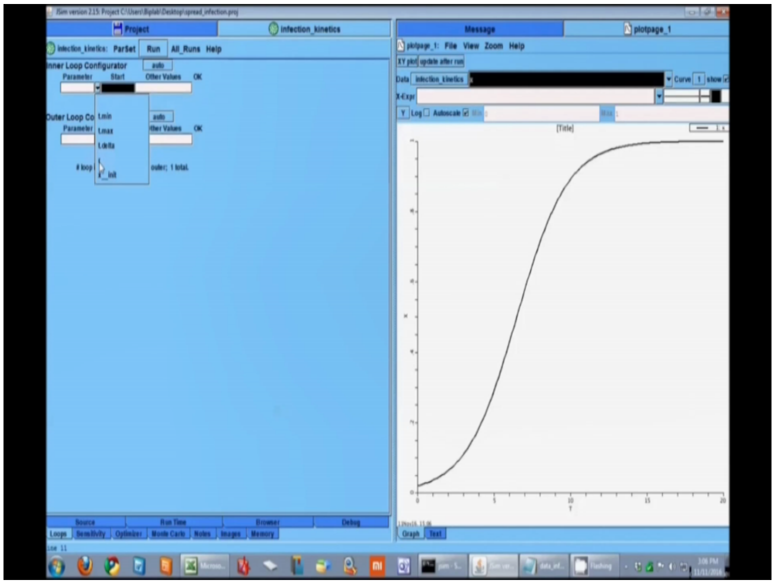
Model Inputs
r .6
x_init .02

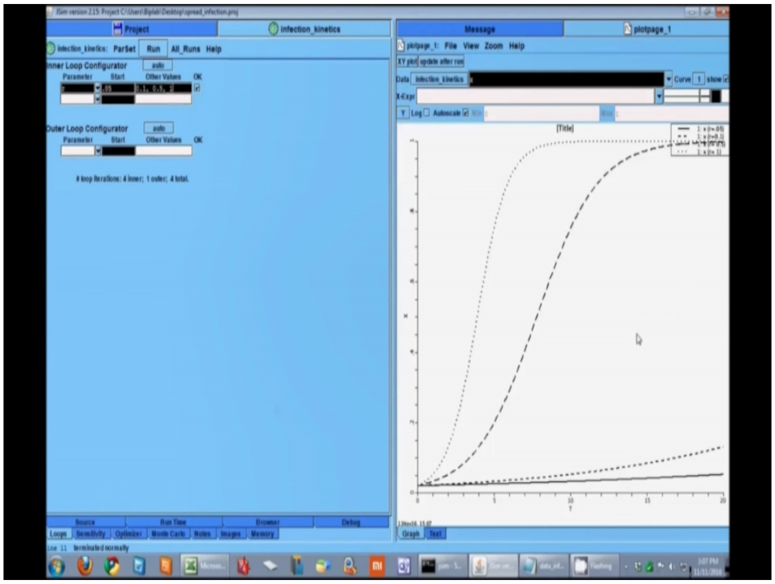
Model Outputs
x(t) .99994
x:t(t) 3.3175E-5

We have removed 1 and we will only show now the main variable x. I will run with default values and I want to see now how if a parameter is changed how the data will change.

(Refer Slide Time: 20:06)







JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj

Inner Loop Configurator

Parameter	Start	Other Values	OK
r	.05	0.1, 0.5, 1	☑

Outer Loop Configurator

Parameter	Start	Other Values	OK

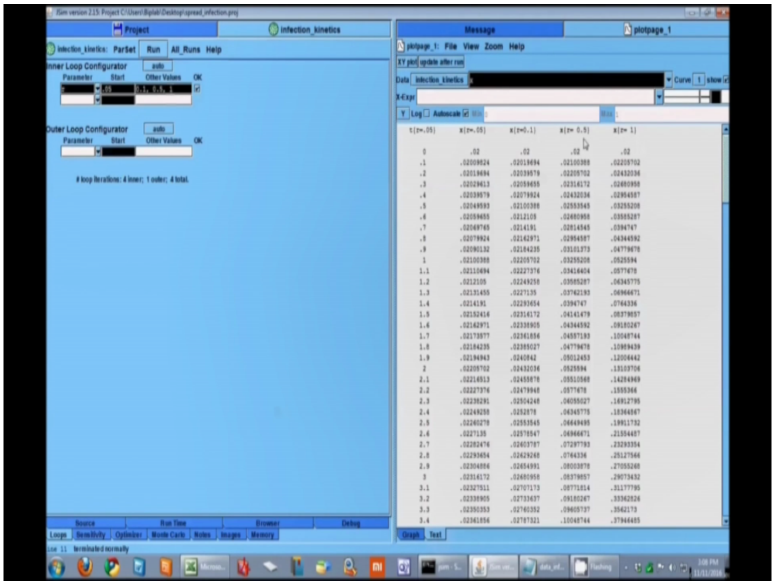
loop iterations: 4 inner; 1 outer; 4 total.

Line 11 terminated normally

So there is loop tab which allow you to check the different value of parameter on your result. So let us choose one parameter from this pull down. You have the parameter R, let me choose that. Let us fix a start value of R i.e. the first value of R that will be used. So it is by default now 0.6 because that is the value in the code. Let me put it as 0.05 and then in other value we put as 0.1, 0.5. So I have 3 values 0.05, 0.1 and 0.5. I want to run this loop and see how the data changes with the change in value of R. So in all run option you have loops run, 3 combat.

So in the graph you can see multiple plots showing the effect of R on the behavior of x. The lowest one, the dark black one is for 0.05 and the upper one, the dotted one is for r equal to 1. Everything else is in between. So in this way you can choose the parameter, set different values of the parameter and use loop run to see how that parameter effect your behavior of the dependent variable.

(Refer Slide Time: 21:40)



JSim version 2.15: Project C:\Users\Biplab\Desktop\spread_infection.proj

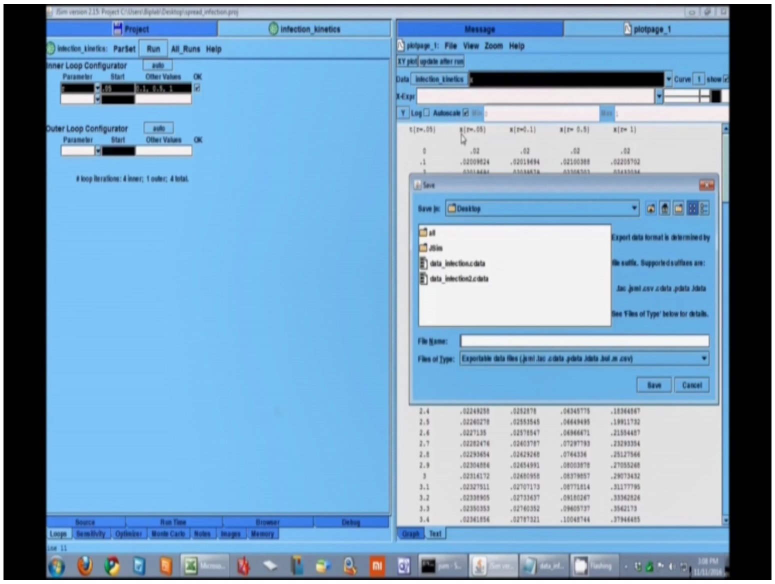
Inner Loop Configurator
Parameter: r Start: .05 Other Values: 0.1, 0.5, 1 OK ☑

Outer Loop Configurator

loop iterations: 4 inner; 1 outer; 4 total.

Data: infection_kinetics Curve 1 Y Log ☐ Autoscale ☑

```
t(r=.05)   x(r=.05)    x(r=0.1)    x(r= 0.5)   x(r= 1)

   0        .02         .02         .02         .02
  .1        .02009824   .02019694   .02100388   .02205702
  .2        .02019694   .02039579   .02205702   .02432036
  .3        .02029613   .02059655   .02316172   .02680958
  .4        .02039579   .02079924   .02432036   .02954587
  .5        .02049593   .02100388   .02553545   .03255208
  .6        .02059655   .0212105    .02680958   .03585287
  .7        .02069765   .0214191    .02814545   .0394747
  .8        .02079924   .02162971   .02954587   .04344592
  .9        .02090132   .02184235   .03101373   .04779678
   1        .02100388   .02205702   .03255208   .0525594
 1.1        .02110694   .02227376   .03416404   .0577678
 1.2        .0212105    .02249258   .03585287   .06345775
 1.3        .02131455   .0227135    .03762193   .06966671
 1.4        .0214191    .02293654   .0394747    .0764336
 1.5        .02152416   .02316172   .04141479   .08379857
 1.6        .02162971   .02338905   .04344592   .09180267
 1.7        .02173577   .02361856   .04557193   .10048744
 1.8        .02184235   .02385027   .04779678   .10989439
 1.9        .02194943   .0240842    .05012453   .12006442
   2        .02205702   .02432036   .0525594    .13103706
 2.1        .02216513   .02455878   .05510568   .14284969
 2.2        .02227376   .02479948   .0577678    .1555366
 2.3        .02238291   .02504248   .06055027   .16912795
 2.4        .02249258   .0252878    .06345775   .18364867
 2.5        .02260278   .02553545   .06649495   .19911732
 2.6        .0227135    .02578547   .06966671   .21554487
 2.7        .02282476   .02603787   .07297793   .23293354
 2.8        .02293654   .02629268   .0764336    .25127566
 2.9        .02304886   .02654991   .08003878   .27055268
   3        .02316172   .02680958   .08379857   .29073432
 3.1        .02327511   .02707173   .08771814   .31177795
 3.2        .02338905   .02733637   .09180267   .33362826
 3.3        .02350353   .02760352   .09605737   .3562173
 3.4        .02361856   .02787321   .10048744   .37946485
```



Save

Save In: Desktop

all
JSim
data_infection.cdata
data_infection2.cdata

Export data format is determined by file suffix. Supported suffixes are: .tac .jsml .csv .cdata .pdata .ldata See 'Files of Type' below for details.

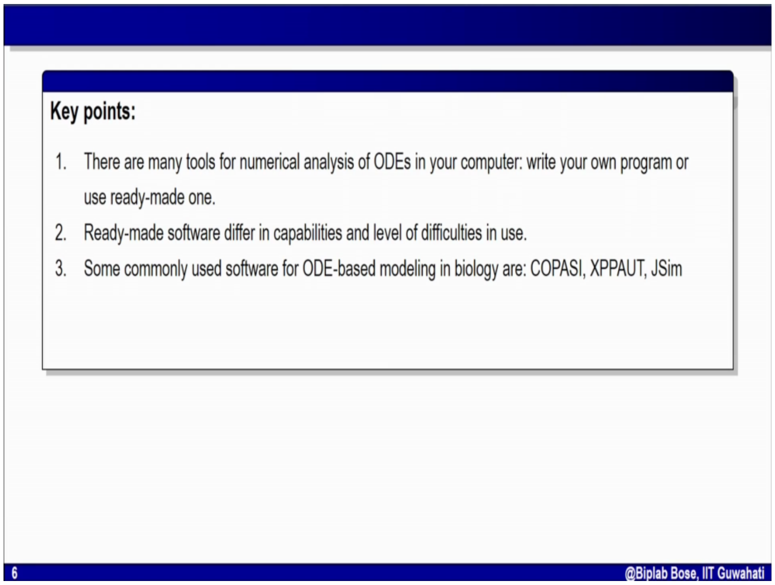
File Name:

Files of Type: Exportable data files (.jsml .tac .cdata .pdata .ldata .bxl .m .csv)

```
t(r=.05)   x(r=.05)    x(r=0.1)    x(r= 0.5)   x(r= 1)

   0        .02         .02         .02         .02
  .1        .02009824   .02019694   .02100388   .02205702
 2.4        .02249258   .0252878    .06345775   .18364867
 2.5        .02260278   .02553545   .06649495   .19911732
 2.6        .0227135    .02578547   .06966671   .21554487
 2.7        .02282476   .02603787   .07297793   .23293354
 2.8        .02293654   .02629268   .0764336    .25127566
 2.9        .02304886   .02654991   .08003878   .27055268
   3        .02316172   .02680958   .08379857   .29073432
 3.1        .02327511   .02707173   .08771814   .31177795
 3.2        .02338905   .02733637   .09180267   .33362826
 3.3        .02350353   .02760352   .09605737   .3562173
 3.4        .02361856   .02787321   .10048744   .37946485
```

You can also see the data text files and you can as usual export that text data in a text file so that you can manipulate and plot in some other software. Here I am saving it as a data_infection_loop.cdata so that data I can use somewhere else.

(Refer Slide Time: 22:04)



Key points:

1. There are many tools for numerical analysis of ODEs in your computer: write your own program or use ready-made one.
2. Ready-made software differ in capabilities and level of difficulties in use.
3. Some commonly used software for ODE-based modeling in biology are: COPASI, XPPAUT, JSim

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So the key points that we have discussed in this module is that there are many software's and programming languages that you can use to model and simulate your ODE based model. You have to choose them depending upon you capabilities and your ease of work. If you are creating very large model then writing down your own program may not be a good idea. May be some software which can handle large model be useful for you. There are many readymade software like Copasi, JSIM which you can use depending upon your utility.

These tool not only allow you to simulate ODE but also allow some other analysis like parameter sensitivity, parameter estimation. These software also allow you to visualize the data and save the data as a text format which you can export and use in some other software. In our course I will advise you to use JSIM for simulating ODE based models and we will discuss in another video how to create JSIM model using JSIM's math model language. Thank You for watching, see you in next module.