injavis Documentation

Release 0.90

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This documentation corresponds to the Injavis Application, written and managed by Michael Engel, as is intended for use within the Glotzer Group.

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SETTING UP INJAVIS ON YOUR COMPUTER

Step 1: Download

The repository for injavis can be found here. If you do not have access to this repo, please contact the admins at glotzerlab-admins@umich.edu.

In your software/programs/desired file, call

git clone <html>

using the html from the top-right corner of the repository page.

Step 2: Compile

Simply call 'make' within the injavis file to compile injavis.

Step 3: Preparing your Computer

In your *bash profile* (".bash_profile"), add a line which assigns the alias "injavis" to the output generated during compiling. It should look something like this:

alias injavis="java -Xmx512m -jar /Users/rosecers/Programs/injavis/bin/injavis.jar"

It is important that there are no spaces preceding or following the equals sign.

Just source your bash profile and then you're ready to go! You're ready for Calling Injavis from the Command Line!

CALLING INJAVIS FROM THE COMMAND LINE

Calling injavis from the command line requires a minimum of two parts on the command line:

1. "injavis"
2. your filename

followed by any number of options found in Command Line Options.

2.1 Command Line Options

When invoking injavis, you may choose to use any of the following options:

2.1.1 Startup Parameters

- **-D <secs>** - Wait/delay for <number> of seconds
- **-f <number>** - Jump to frame <number>
- **-s <module> <par> <value>** - Set parameter <par> of <module> to <value> [1]
- **-S <file>** - Load external simulation from <file>
- **-x** - Maximize window at startup

2.1.2 Modifying Visuals

- **-a <num>** - Use *ambient occlusion* [2] with <num> runs
- **-d <width> <height>** - Set window dimensions to (<width>, <height>)
- **-N <number>** - Multiply box to approximately <number> particles
- **-r** - Resize and center for full visibility

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[1] A full list of modules and functions can be found in Available Modules (and how to use them)

[2] *Ambient Occlusion* is shading/rendering technique that allows the user to see greater depth and exposition, as if under environmental/natural lighting.

2.1.3 Analysis and Outputting Data

- **-F <img_in> <img_out> <i>** - Fourier transform <img_in> with intensity <i> and outputs to <img_out>

- **-M <module>** <file> - Save data from <module> to <file>

- **-o <file>** - Write single HOOMD-Blue snapshot to <file>

- **-O <file>** - Write multiple snapshots to <file>

- **-R <min> <max>** - Set RDF range to [min, max]

2.1.4 Actions and Controls

- **-A <module> <item>** - Menu action of <item> in <module>

  This option can call functions within any of the injavis modules [2]:

  These options need to be written with their exact syntax, but case doesn't matter. If the function is more than one word, it needs to be called in quotation marks.

- **-h or -?** - Display all injavis command line options

- **-m <message>** - Send a <message> to simulation

- **-q** - Quit after executing previous commands

2.2 Input Formats

Let's be honest, this is the easiest way to cause errors in injavis. Injavis will read pos-format files (.posextension). Most pos dump (i.e.dump.pos() in hoomd) functions will out put the file in the correct format, but let's delve a bit more. . .

2.2.1 What kind of shapes can you make? And how?

Shape	Filename	pos syntax (all on one line) [3]
Arrow	Arrow	def A "arrow *length color*"
Bond	BondShape	def A "bond length color*"
Box Segment	BoxSegmentShape	No definition found, shape is most likely no longer used. (codeword: boxsegment)
Connections	ConnectionShape	def A "connection *diameter color*"
Cylinder	CylinderShape	def A "cyl diameter height color*"
Ellipsoid	EllipsoidShape	def A "ellipsoid *diameter1 diameter2 diameter3*"
Janus Ellipsoid	JanusEllipsoidShape	def A "jellipsoid *diameter1 diameter2 diameter3 patch_diameter1 patch_diameter1 patch_diameter3 overlap_radius*"
Janus Sphere	JanusSphereShape	def A "jsphere *diameter patch_diameter overlap_radius*"
Multisphere	MultiSphereShape	def A "sphere_union *num_spheres diameter1 center1 color1 diameter2 ...* "
Pacman [4]	PacmanShape	def A "pacman *diameter1 diameter2 separation_radius*"
Polygon n	PolygonShape	No definition found, shape is most likely no longer used. (codeword: poly)
Polyhedron	PolyhedronShape	def A "poly3d *num_vertices vertex1 vertex2 vertex3 ... color*"
Polyhedron Sphere [5]	PolyhedronSphereShape	def A "spoly3d *rounding num_vertices vertex1 vertex2 vertex3 ... color*"
Polyhedron Vertices	PolyhedronVerticesShape	No definition found, shape is most likely no longer used. (codeword: polyV)
Roly Poly Shape	RolyPoly3Shape	No definition found, shape is most likely no longer used. (codeword: rolypoly3)
Sphere	SphereShape	def A "sphere *radius color*"
Spheropolyhedron	SpheroPolyhedronShape	def A "spoly3d *rounding num_vertices vertex1 vertex2 vertex3 ... color*"
Sphinx	SphinxShape	def A "sphinx 0 1. *num_spheres diameter1* [6] *center1 color1 diameter2* [7] *center2 color2...*"
Triblock Sphere	TriblockSphereShape	def A "trisphere *main_radius percentage_center_band color_patches color_main_sphere*"

2.2.2 More to do with POS files here

Simulation data can be put into the POS file under the heading #[data] followed by all variable names. Data can be entered in corresponding spaces in the following lines.

OPERATING THE INJAVIS WINDOW

3.1 Available Modules (and how to use them)

Injavis' modules can be found in dropdown menus in the interactive window, and also have optional visual displays in the window [1].

These are the current available modules and subgroups of the functions:

3.1.1 File

These are the functions available in the file module.

Input/Output

- **Load ... (Ctrl+L)**: Prompts the load menu
- **Save ... (Ctrl+S)**: Prompts the save menu
- **Save all Frames ...**: Prompts the save menu for all frames

Frame Progression

- You may move the frame by the following functions: **First Frame**, **-25 Frames**, **-1 Frame**, **+1 Frame**, **+25 Frames**, **Last Frame**:

Play Controls

- **Play Movie (S)**: Play the frames of the simulation in order
- **Frames Per Second**: Change the speed of the movie (options: 1, 2, 5, 10, 20, 50, 100)
- **Loop**: Loop the movie

File Progression

- You may change the file using the following functions: **First File**, **25 Files**, **1 File**, **Current File**, **+1 File**, **+25 Files**, **Last File**

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[1] On PC's, you must execute all "Ctrl + " shortcuts with the right Ctrl key.

Quit

- **Quit (Q)**: Quit the current window

3.1.2 Edit

- **Add (A)**: Add particles to the simulation (Note: Add and Delete are not inverse functions)
- **Delete (D)**: Delete particles from the simulation
- **Invert Selection (I)**: Select the non-selected particles, and deselect the selected

Colors

- **Color: Red (Ctrl+R)**: Change all (or selected) particles to Red
- **Color: Green (Ctrl+G)**: Change all (or selected) particles to Green
- **Color: Blue (Ctrl+B)**: Change all (or selected) particles to Blue
- **Color: Random (Ctrl+A)**: Change all (or selected) particles to a random color
- **Copy Color (1->2)**: Take color from particle 1, and copy it to particle 2

Modes [2]

- **Mode: Standard**: View simulation in standard viewing mode
- **Mode: Show Center (C)**: View simulation particles by center of particle only
- **Mode: Edit Visibility (E)**: Make simulation particles selectable in order to delete desired particles
- **Mode: Translate (T)**: Mode to move selection by a finite translation
- **Mode: Mark 1 (1)**: Mode to mark particle(s) '1' for further observation
- **Mode: Mark 2 (2)**: Mode to mark particle(s) '2' for further observation
- **Mode: Mark 3 (3)**: Mode to mark particle(s) '3' for further observation

3.1.3 View

- **Resize and Center (0)**: Resize and center the particle box
- **Restore (V)**: Restore original view
- **Record (Ctrl+V)**: Record the view (output is questionable)
- **Set Current View**
- **Center Particles (Ctrl+P)**
- **Relative to Observer**: Set view relative to observer
- **Show (Shift+V)**: Show view display box
- You can choose to enable/disable: **Dragging in x-direction (Ctrl+X)**, **Dragging in y-direction (Ctrl+Y)**
- You can choose to **View along x-axis (X)**, **View along y-axis (Y)**, **View along z-axis (Z)**

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[2] For all modes, pressing the shortcut key again will clear any selection.

- You can choose to **Rotate up 90 Degrees**, **Rotate down 90 Degrees**, **Rotate left 90 Degrees**, or **Rotate right 90 Degrees**

3.1.4 Simulation(s in Injavis)

Injavis is able to work interactively with incsim simulations, and these options are meant for these simulations.

Controls

- **Load (Ctrl+M)**: Prompts the load menu
- **(Re)Initialize (Ctrl+I)**: Initialize a new simulation in an interactive session. This will also allow you to keep all changed options in the new simulation
- **Protocol**: Specify the pos file for exporting further trajectory data
- **Show (Shift+S)**: Show the simulation display box
- **Run (S)**: Play the frames of the simulation in order
- **Send Message (M)**: Send a message or command to the simulation

Particle Data

- **Average Particle Data**: Calculate Average Particle Data
- **Set Reference Configuration**
- **Remove Reference Configuration**

3.1.5 Object

- **About (F1)**

List of Simulation Elements

Allows you to turn on/off simulation elements.

Includes: **box (Ctrl+Shift+X)**, **particles (Ctrl+Shift+D)**

Rendering

- **Show Edges**: draw edges of all polygons with thin black lines
- **Perspective**: gives distance perspective to the particles
- **Add Fog**: objects further away are drawn brighter
- **Anti-aliasing**: prevents aliasing by representing a high-resolution image at a lower resolution
- **Anaglyph (3D)**: a function which induces pseudo-3D effect by filtering the image to induce a stereoscopic effect

3.1.6 Particles

- **Show (Shift+P)**: Allows you to turn on/off the particle display box

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3.1.7 Data

This module presents the specified simulation data on a plot at the bottom of the window.

This only works in two cases:

1. Interactive Simulations
2. When data is defined within the pos file

3.1.8 Box

- **Duplicate Box (Ctrl+D)**: duplicate the number of unit cells in each direction (i.e. 1 unit cell -> 8)
- **Fit in Box (Ctrl+F)**: fit all particles inside the box
- **Delete Outside**: delete any particles outside the box

Set Box

This is used for unit cell determination and requires cylinder view be enabled and bonds be calculated.

Each of these options takes the average vector of bonds to generate the axis vector for the given direction:

- **Set Unit Cell X (LDF)**
- **Set Unit Cell Y (LDF)**
- **Set Unit Cell Z (LDF)**
- **Set Box (Unit Cell)**
- **Set Box (1+2+2+2)** - Mark a particle 1 and three others as 2 to generate a unit cell box from them.

3.1.9 RDF

The radial distribution function is a good way of analyzing the crystal structure, as it is a measure of nearest neighbors.

For more info, feel free to visit the 'wikipedia page on RDF. <https://en.wikipedia.org/wiki/Radial_distribution_function>'_.

- **Save**: Save the RDF
- **Show (Shift+R)**: Show/Unshow the RDF display box

Calculation

- **Calculate (R)**
- **Auto**
- **Average**

Modify RDF

- **Range**: Choose RDF range from 1, 2, 5, 10, 20, 50, 100
- **Detect Peak**
- **Add Voronoi Cells** (see 'wikipedia page <https://en.wikipedia.org/wiki/Voronoi_diagram>'_)
- **Enable Cylinder View (LDF) (Ctrl+C)**: Change binning process for RDF calculation
- **Cylinder Radius**: Choose cylinder radius from: 0.01, 0.02, 0.05, 0.1, 0.2, 0.5, 1
- **Periodic Boundary Conditions**: Turn on/off periodic boundary conditions

3.1.10 Bonds

- **Save**: Save bond order diagram
- **Show (Shift+B)**: Show bond order display box

Calculation

- **Calculation (B)**: Calculate Bond Order Diffraction pattern for the crystal cell
- **Auto**
- **Average**
- **Find Symmetric Orientation (Local) (O)**: Searches for local high symmetry direction
- **Find Symmetric Orientation (Global) (Ctrl+O)**: Searches for highest symmetry direction

Parameters

- **Intensity**: Choose intensity of pattern, from 1-10
- **Size**: Choose relative resolution of the bond order diagram (higher size is higher resolution)
- **Zoom (Command+Shift+X)**
- **Peak Width**
- **Show Center**: Turn on/off center marker on bond order diagram
- **Show Grid**: Show grid on bond order diagram

Bond Order View

- **Parallel Projection**: Histogram of bond order diagram projected on the surface of a sphere
- **Stereographic Projection**: Histogram of bond order diagram projected from a sphere onto a plane (mainly used by crystallographers)
- **Map Projection**: Histogram of bond order diagram projected on a map surface using Mollweide Projection (see 'wikipedia page <https://en.wikipedia.org/wiki/Mollweide_projection>'_)

Analysis

- **Analyze Symmetry**: Show mirror planes, 2,3,4,and 6-fold axes
- **Include Quasi-Symmetries**: Turn on/off quasi-symmetries
- **Add Markers**
- **Delete Markers**

3.1.11 Diffraction

- **Save**
- **Show (Shift+F)**

Calculation

- **Calculation (F)**: Calculates X-Ray Diffraction pattern. More info on the 'XRD wikipedia page. <https://en.wikipedia.org/wiki/X-ray_crystallography#X-ray_analysis_of_crystals>'_.
- **Auto**
- **Average**

Parameters

- **Intensity**: Choose diffraction pattern intensity from 1-10
- **Size**: Choose image resolution
- **Zoom**
- **Peak Width**

Mode

- **Diffraction Mode**: Shows diffraction pattern
- **Filter Mode**: Filters out extraneous signals for clearer pattern
- **Autocorrelation Mode**: Correlates signals into patterns
- **Black & White**: Turn on/off color
- **Invert Color**
- **Flat Sample**: Show diffraction pattern on a flat sample

3.1.12 Network

Analyze the network of bonds.

- **Show (Shift+N)**: Show the network display box in the window
- **Save**: Save the network display

Calculation

- **Calculate (N)**: Calculate the network coordination based on the mode
- **Auto**: Update automatically
- **Average**
- **Number of Bins**: Increase the number of data points possible for each particle (graphically)

Mode

- **Bonds per Particle**
- **Angle between Bonds**
- **Multipole Expansion**: Expands bond order diagram via spherical harmonic expansion. (see 'wikipedia page <https://en.wikipedia.org/wiki/Multipole_expansion>'_)
- **Cluster Sizes**

Clusters

- **Find Cluster Centers**
- **Delete Small Clusters**

Shapes

- **Find Triangles**
- **Find Squares**
- **Find Pentagons**
- **Find Hexagons**
- **Find Tetrahedra**
- **Find Octahedra**
- **Add Coordination Polyhedra**

3.2 Injavis Shortcuts

3.2.1 Injavis Simulation Shortcut Library - By Letter

- **A** - add particles
- **B** - calculate bonds
- **C** - show center
- **D** - delete particles
- **E** - edit visibility mode
- **F** - calculate diffraction pattern

- **I** - invert selection
- **M** - send message
- **N** - calculate network
- **O** - find symmetric orientation (local)
- **R** - calculate RDF
- **S** - play, run
- **T** - translate mode
- **V** - restore original frame
- **X** - view along x-axis
- **Y** - view along y-axis
- **Z** - view along z-axis
- **0** - resize and center particles
- **1** - mark mode (1)
- **2** - mark mode (2)
- **3** - mark mode (3)

Control + ___

- **A** - make particles random color
- **B** - make particles blue
- **C** - enable cylinder view (LDF)
- **D** - duplicate particles
- **F** - fit particles into box
- **G** - make particles green
- **I** - initialize system
- **L,M** - load simulation file
- **O** - find symmetric orientation (global)
- **P** - center particles
- **Q** - quit simulation window
- **R** - make particles red
- **S** - save simulation
- **V** - record simulation
- **X** - drag along x-axis
- **Y** - drag along y-axis

Shift + ___

- **B** - show bonds module display box
- **D** - show data module display box
- **F** - show diffraction module display box

- **N** - show network module display box
- **P** - show particle module display box
- **R** - show RDF module display box
- **S** - show simulation module display box
- **V** - show view module display box
- **Ctrl+Shift+X** - turn on/off box display
- **Ctrl+Shift+D** - turn on/off particle display
- **Command+Shift+X** - zoom on module display box

3.2.2 Injavis Simulation Shortcut Library - By Module

File

- **Ctrl+L** - load simulation file
- **Ctrl+S** - save simulation
- **S** - play, run
- **Ctrl+Q** - quit simulation window

Edit

- **A** - add particles
- **D** - delete particles
- **I** - invert selection
- **Ctrl+R** - make particles red
- **Ctrl+G** - make particles green
- **Ctrl+B** - make particles blue
- **Ctrl+A** - make particles random color
- **C** - show center
- **E** - edit visibility mode
- **T** - translate mode
- **1** - mark mode (1)
- **2** - mark mode (2)
- **3** - mark mode (3)

View

- **0** - resize and center particles
- **V** - restore original frame
- **Ctrl+V** - record simulation

- **Ctrl+P** - center particles
- **Ctrl+X** - drag along x-axis
- **Ctrl+Y** - drag along y-axis
- **X** - view along x-axis
- **Y** - view along y-axis
- **Z** - view along z-axis
- **Shift+V** - show view module display box

Simulation

- **Ctrl+M** - load simulation file
- **Ctrl+I** - initialize system
- **S** - play, run
- **M** - send message
- **Shift+S** - show simulation module display box

Objects

- **Ctrl+Shift+X** - turn on/off box display
- **Ctrl+Shift+D** - turn on/off particle display
- **F1** - About

Particles

- **Shift+P** - show particle module display box

Data

- **Shift+D** - show data module display box

Box

- **Ctrl+D** - duplicate particles
- **Ctrl+F** - fit particles into box

RDF

- **R** - calculate RDF
- **Ctrl+C** - enable cylinder view (LDF)
- **Shift+R** - show RDF module display box

Bonds

- **B** - calculate bonds
- **O** - find symmetric orientation (local)
- **Ctrl+O** - find symmetric orientation (global)
- **Command+Shift+X** - zoom on module display box
- **Shift+B** - show bonds module display box

Diffraction

- **F** - calculate diffraction pattern
- **Shift+F** - show diffraction module display box

Network

- **N** - calculate network
- **Shift+N** - show networks module display box

FOUR

OUTPUTTING DATA FROM INJAVIS

There is a glog post by Josh Anderson on making movies from injavis. I'll distill it here.

4.1 Ouput your simulation data to images

- Take your simulation data and convert it to images:

  injavis yourfile.pos -O imagename.png

    - For each frame in your simulation, injavis will append a frame number between your image name and .png, i.e. imagename.png -> imagename001.png.

    - If it is a diffraction pattern, use *injavis yourfile.pos -f FRAME [-s Diffraction option value] -M Diffraction imagename.png*

- Save all frames from within simulation window

- File -> Save All

- In your bash window, injavis will output a line for each frame signifying it has been saved. After these lines, it will output an ffmpeg (see below) command which you can run to convert these images into a movie.

4.2 Making Movies

- Use **ffmpeg** to make a movie from image files

    - Install ffmpeg from macports. (There is documentation on ffmpeg here)

    - Run *ffmpeg -qscale 5 -r 20 -i imagename%04d.png moviename.mpg*

        - options:

        - **qscale**: fixed quality scale, between 1-31 (1 being best)

        - **r**: frame rate in frames per second

        - **i**: input files. If they include serialized numbers, then the inclusion of %0xd will indicate that there are x numbers in that placeholder.

    - More options can be found here.

- Use **QuickTime Player 7 Pro** to make a movie from image files

    - Select "File > Open Image Sequence" and select the first image of the sequence.

    - In the next menu, select the frame rate.

- Select "File > Export".
- In the "Export" dropdown menu select "Movie to QuickTime Movie".
- Click on the "Options" button.
- Under "Settings" choose compression type H.264. Choose quality as desired.
- Save file using the ending ".mpg".
- Quick time suggests the ending ".mov", but H.264 (and MPEG-2) codecs really create a ".mpg" file.

FIVE

OTHER COOL THINGS TO DO IN INJAVIS!

5.1 Find the unit cell

5.1.1 Part 1

1. Load the file in injavis

2. Hit options **R**, **B**, **Ctrl+P** (RDF, bond order diagram, center particles)

3. Select the first peak in the RDF

4. Option **Ctrl+O** (find best orientation)

5. Option **Ctrl+C** (enable cylinder/LDF view)

5.1.2 Part 2

6. Find periodicity along viewing direction (mark peak at end of repeat unit in RDF)

7. Define periodicity as x (Menu "Box" > "Set Unit Cell X (LDF)")

8. Option **Alt+LeftArrow** (rotate particles to the left by 90°)

9. Find periodicity along viewing direction (mark peak at end of repeat unit in RDF)

10. Define periodicity as y (Menu "Box" > "Set Unit Cell Y (LDF)")

11. Option **Alt+ArrowDown** (rotate particles down by 90°)

12. Find periodicity along viewing direction (mark peak at end of repeat unit in RDF)

13. Define periodicity as z (Menu "Box" > "Set Unit Cell Z (LDF)")

5.1.3 Part 3

14. Option **Ctrl+C** (switch back to RDF mode)

15. Change RDF range to 1 (Menu "RDF" > "Range" > "1")

16. Option **Shift+R** (display RDF)

17. Mark positions without neighbors corresponding to unit cell vectors [1] & (Click on "N0" particle in "Particle(s)" selection - top left)

18. Option **D** (delete marked particles)

19. Mark first peak in RDF

5.1.4 Part 4

20. Option **Shift+N** (show network)

21. Display cluster sizes ((Menu "Network" > "Cluster Sizes")

22. Get overview over featured bins (Menu "Network" > "Cluster Sizes")

23. Select too-small bins only (Menu "Network" > "Number of Bins" > <smaller number>)

24. Delete too-small clusters ((Menu "Network" > "Delete Small Clusters")

25. Collapse clusters to points (Menu "Network" > "Find Cluster Centers")

26. Option **Shift+N** (hide network data)

27. Option **Shift+R** (hide RDF)

28. Save pos files (**Ctrl+S**)