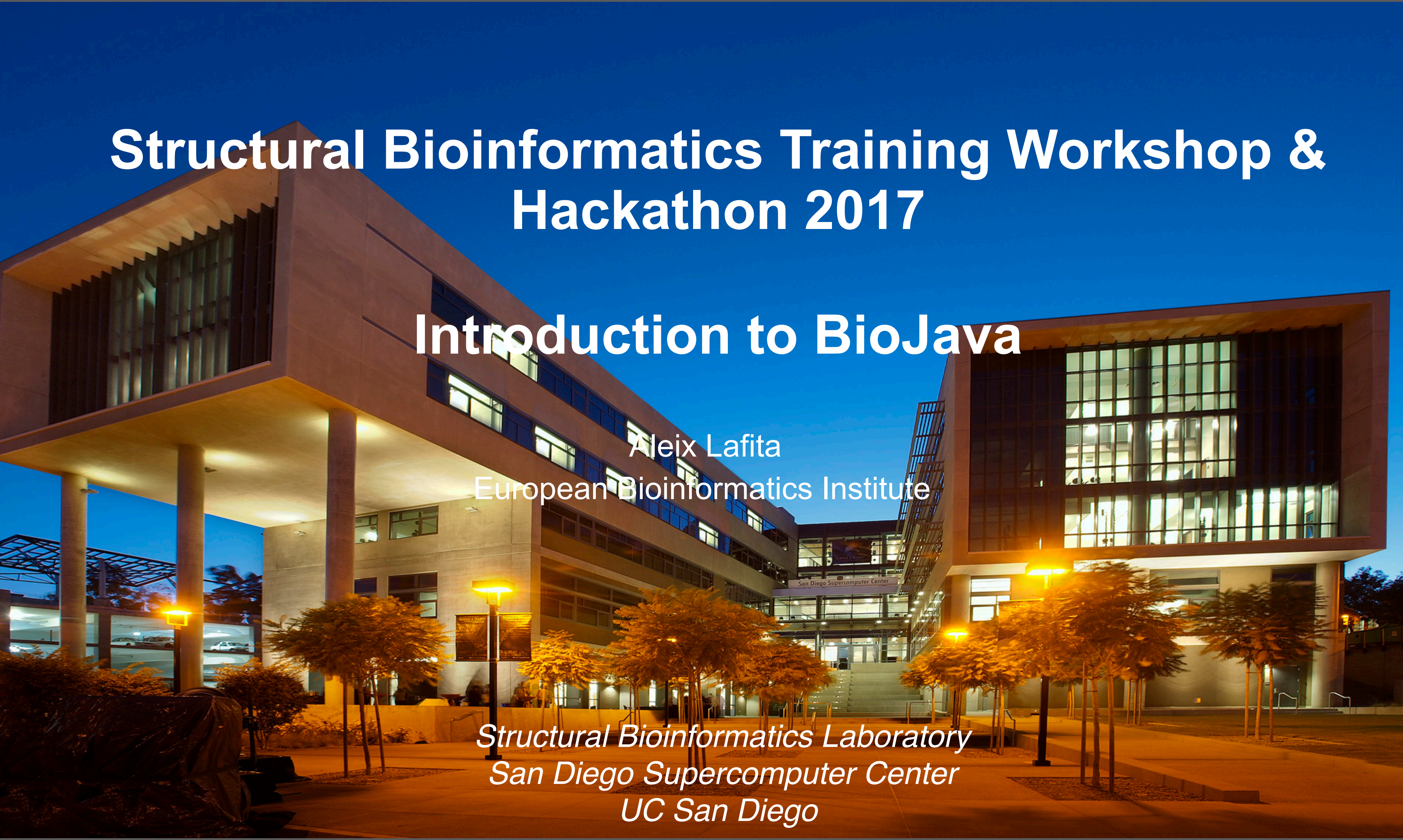

Structural Bioinformatics Training Workshop & Hackathon 2017

Introduction to BioJava

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Structural Bioinformatics Laboratory
San Diego Supercomputer Center
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SDSC SAN DIEGO SUPERCOMPUTER CENTER

RCSB PDB

UC San Diego

PART 1

BioJava Project

History

Resources

Setup

BioJava

BioJava is an **open-source** project dedicated to providing a **Java framework** for processing **biological data**

File parsers

- FASTA
- PDB
- MMCIF
- MMTF

Data models

- Biological sequences
- Protein structures

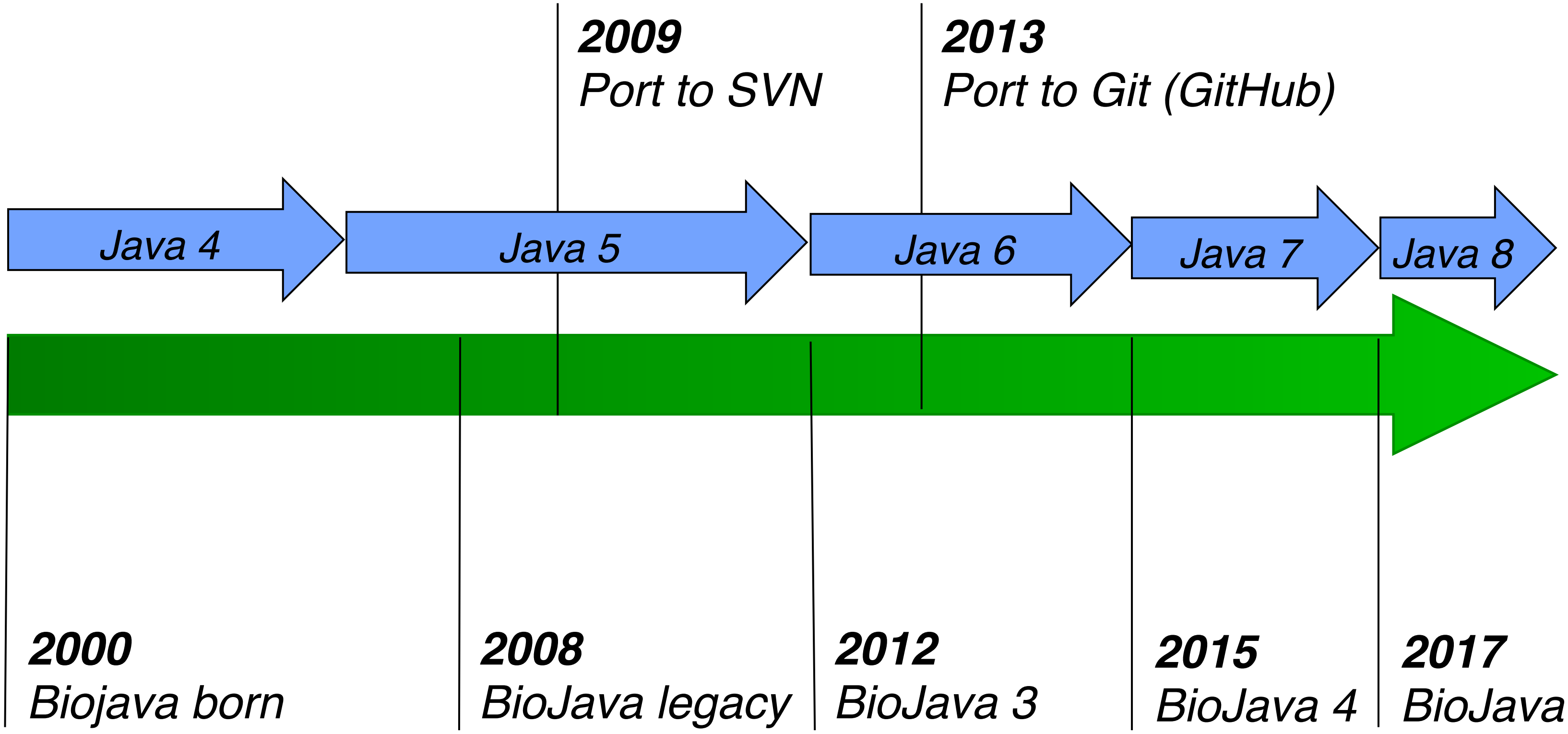
Algorithms

- Sequence and structure alignment
- DSSP
- Symmetry

Resources

- BLAST
- Protein domains: SCOP, CATH, ECOD

History of BioJava



2009
Port to SVN

2013
Port to Git (GitHub)

Java 4

Java 5

Java 6

Java 7

Java 8

2000
Biojava born

2008
BioJava legacy

2012
BioJava 3

2015
BioJava 4

2017
BioJava 5

Pocock et al

Holland et al

Prlić et al

BioJava Resources

Website: https://biojava.org

Source code: https://github.com/biojava/biojava/

Wikipedia: https://en.wikipedia.org/wiki/BioJava

General information about the project

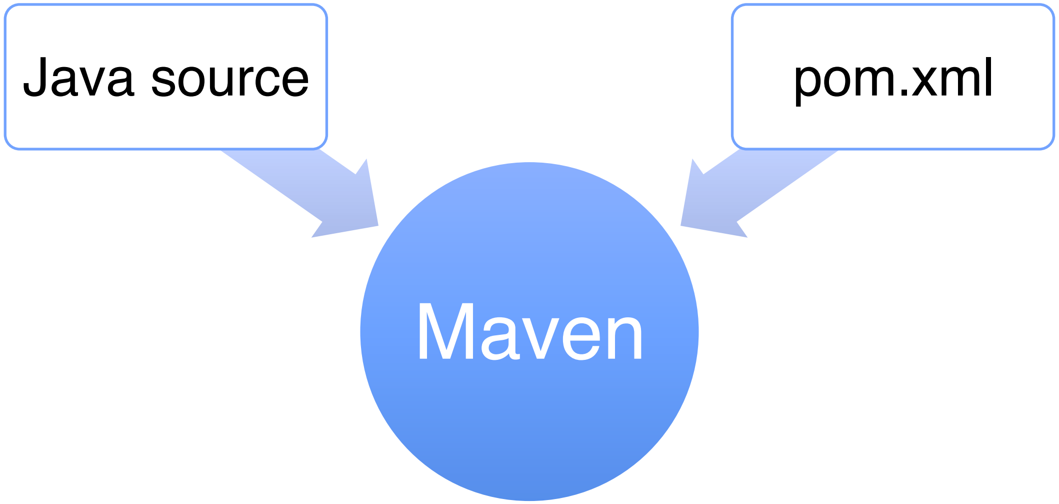
Tutorial: https://github.com/biojava/biojava-tutorial

Educational introduction into the tools provided by BioJava

Cookbook: http://biojava.org/wiki/BioJava:CookBook

Collection of “How do I…?” recipes for common tasks

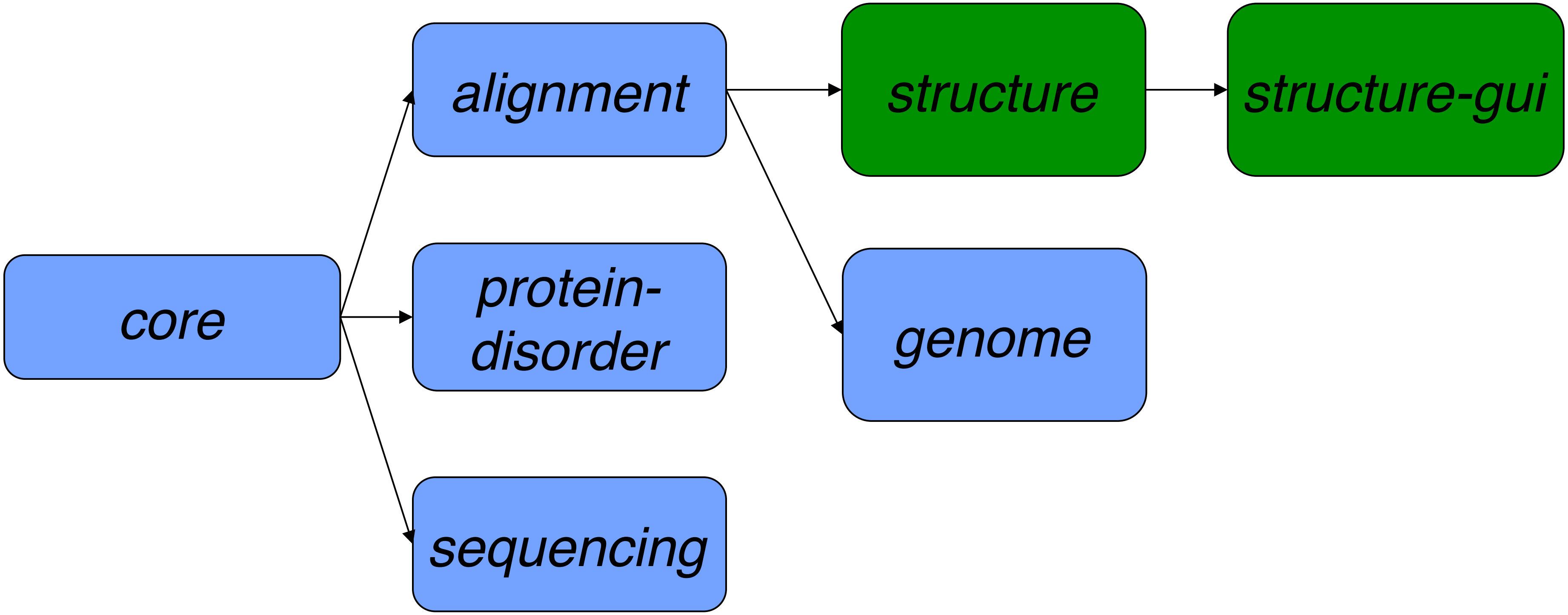
Setting up BioJava



- **Project Object Model (POM):** XML file that contains information about the project and configuration details

Setting up BioJava

- **BioJava modules**

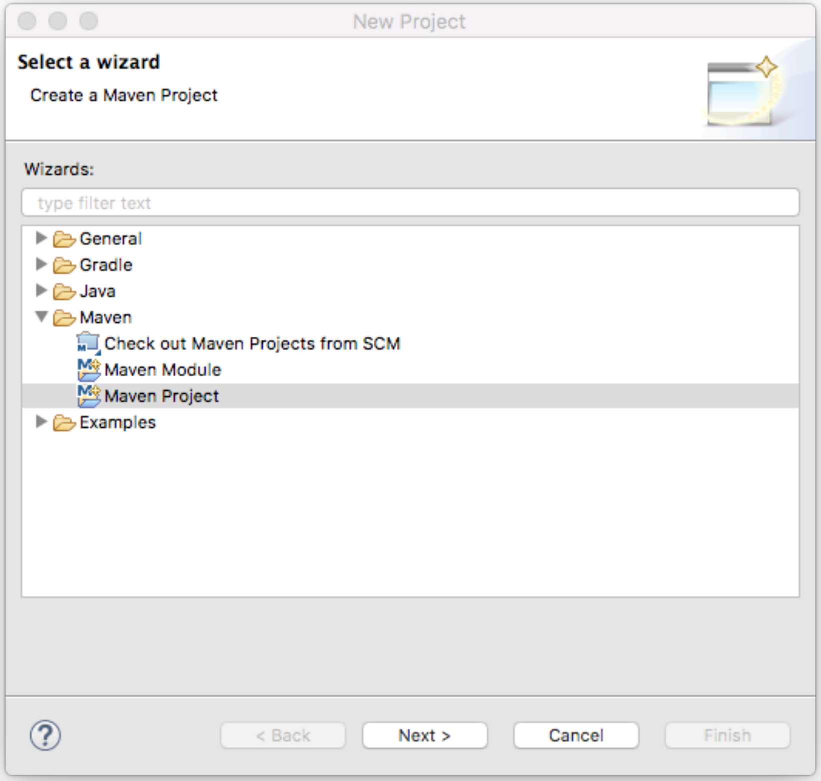


Demo 1

- Create a new Maven repository in Eclipse

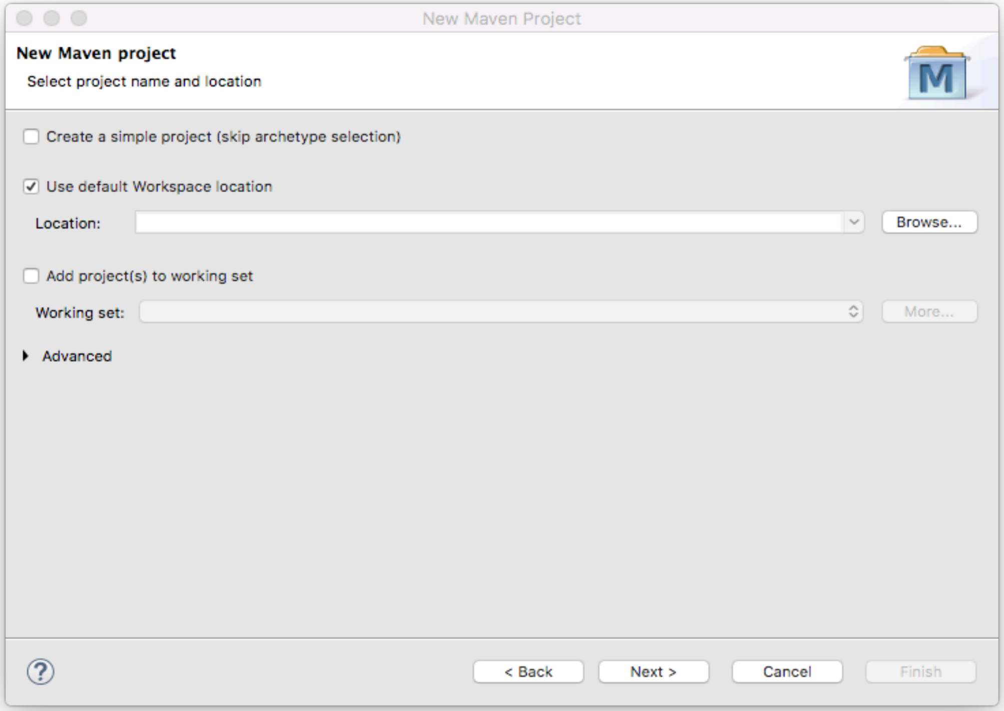
Demo 1

- **Create a new Maven repository in Eclipse**
  1. File > New > Project
  2. Maven Project



Demo 1

- **Create a new Maven repository in Eclipse**
  1. File > New > Project
  2. Maven Project
  3. Use defaults



New Maven Project

New Maven project

Select project name and location

☐ Create a simple project (skip archetype selection)

☑ Use default Workspace location

Location:

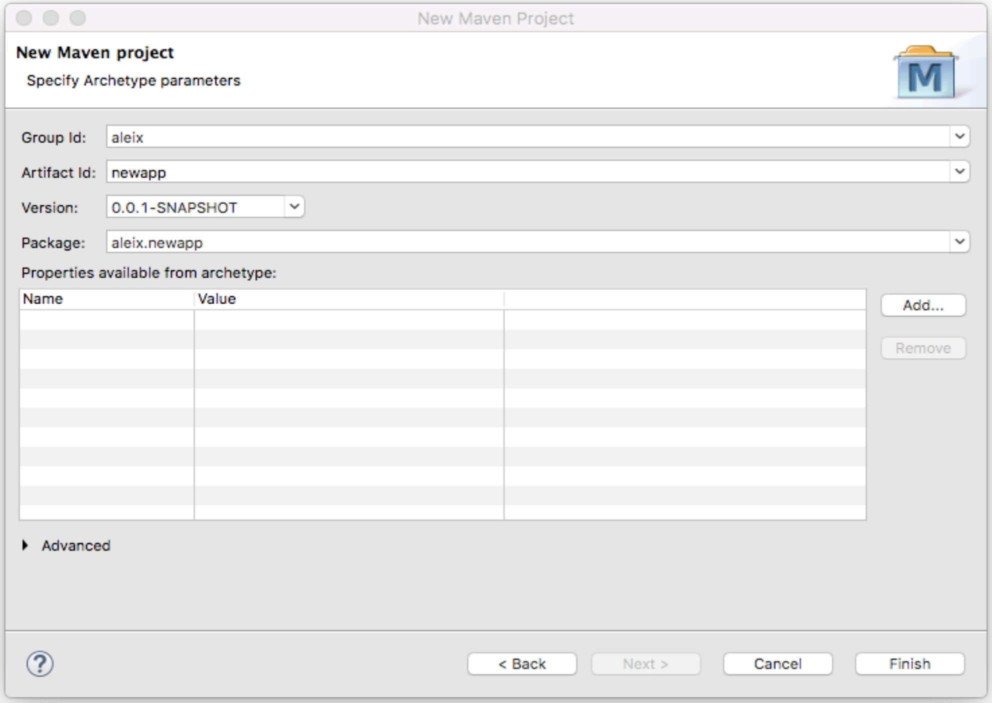
☐ Add project(s) to working set

Working set:

▸ Advanced

Demo 1

- **Create a new Maven repository in Eclipse**
  1. File > New > Project
  2. Maven Project
  3. Use defaults
  4. Choose your group and project id



New Maven Project

New Maven project

Specify Archetype parameters

Group Id: aleix

Artifact Id: newapp

Version: 0.0.1-SNAPSHOT

Package: aleix.newapp

Properties available from archetype:

Name	Value

Problem 1

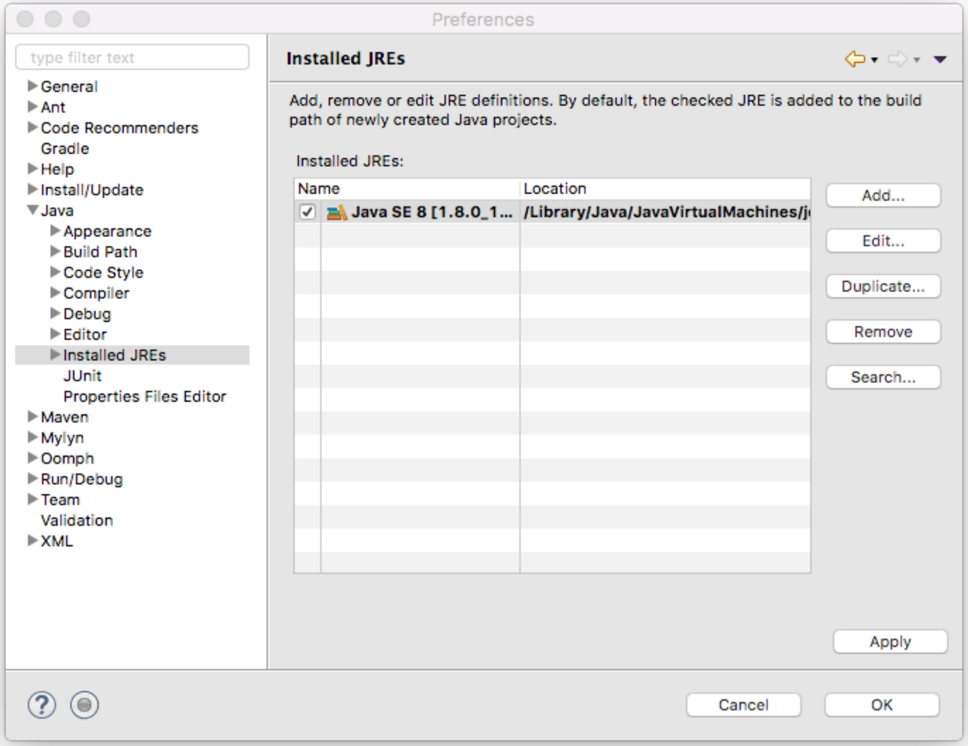
- **Configure the new Maven repository and add the BioJava dependency**
  - **Task 1**: fill in the URL field (replace the default URL)
  - **Task 2**: configure the Java 8 JDK. Insert these properties in the POM:

```
<jdk.version>1.8</jdk.version>
<maven.enforcer.jdk-version>1.8</maven.enforcer.jdk-version>
<maven.compiler.source>1.8</maven.compiler.source>
<maven.compiler.target>1.8</maven.compiler.target>
```

  - **Task 3**: insert the *biojava-stucture-gui* dependency (hint: https://github.com/biojava/biojava-tutorial/blob/master/installation.md)
  - **Task 4:** ensure BioJava version is the latest (5.0.0-alpha8)

Demo 1

- **Configure the BioJava environment**
  1. Eclipse > Preferences > Java > Installed JREs
  2. Edit…



Installed JREs

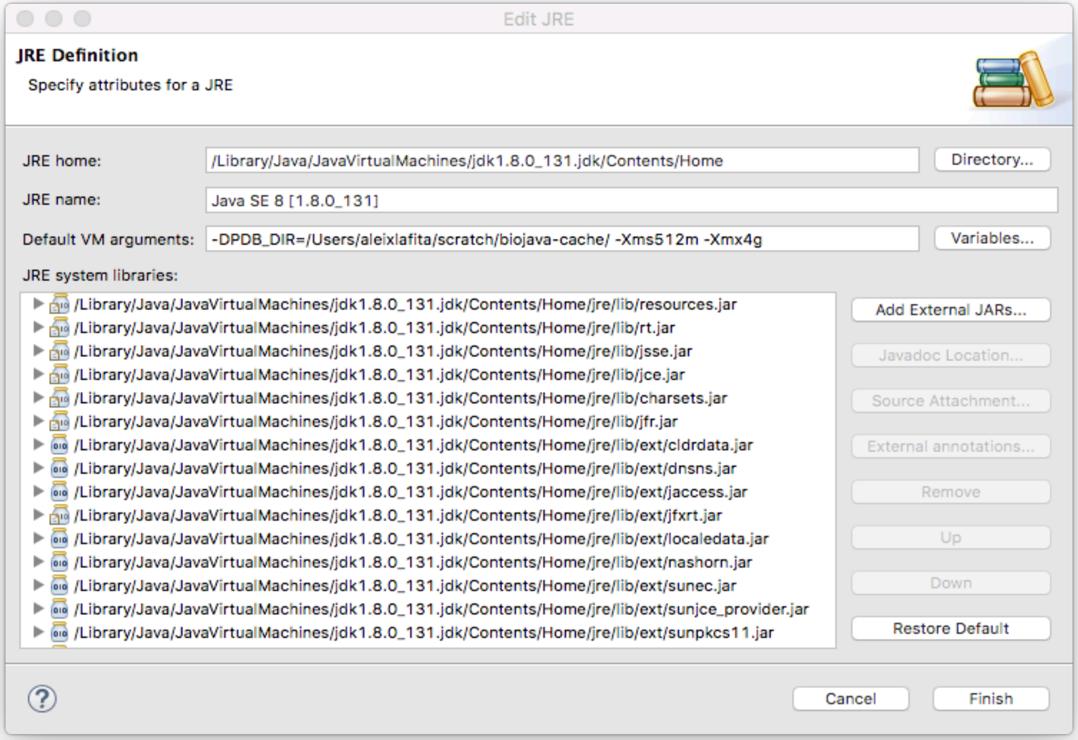
Add, remove or edit JRE definitions. By default, the checked JRE is added to the build path of newly created Java projects.

Installed JREs:

Name	Location
☑ Java SE 8 [1.8.0_1...	/Library/Java/JavaVirtualMachines/j

Demo 1

- **Configure the BioJava environment**
  1. Eclipse > Preferences > Java > Installed JREs
  2. Edit…
  3. Add -DPDB_DIR= directory



Edit JRE

JRE Definition

Specify attributes for a JRE

JRE home: /Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home

JRE name: Java SE 8 [1.8.0_131]

Default VM arguments: -DPDB_DIR=/Users/aleixlafita/scratch/biojava-cache/ -Xms512m -Xmx4g

JRE system libraries:

```
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/resources.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/rt.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/jsse.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/jce.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/charsets.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/jfr.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/ext/cldrdata.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/ext/dnsns.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/ext/jaccess.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/ext/jfxrt.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/ext/localedata.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/ext/nashorn.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/ext/sunec.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/ext/sunjce_provider.jar
/Library/Java/JavaVirtualMachines/jdk1.8.0_131.jdk/Contents/Home/jre/lib/ext/sunpkcs11.jar
```

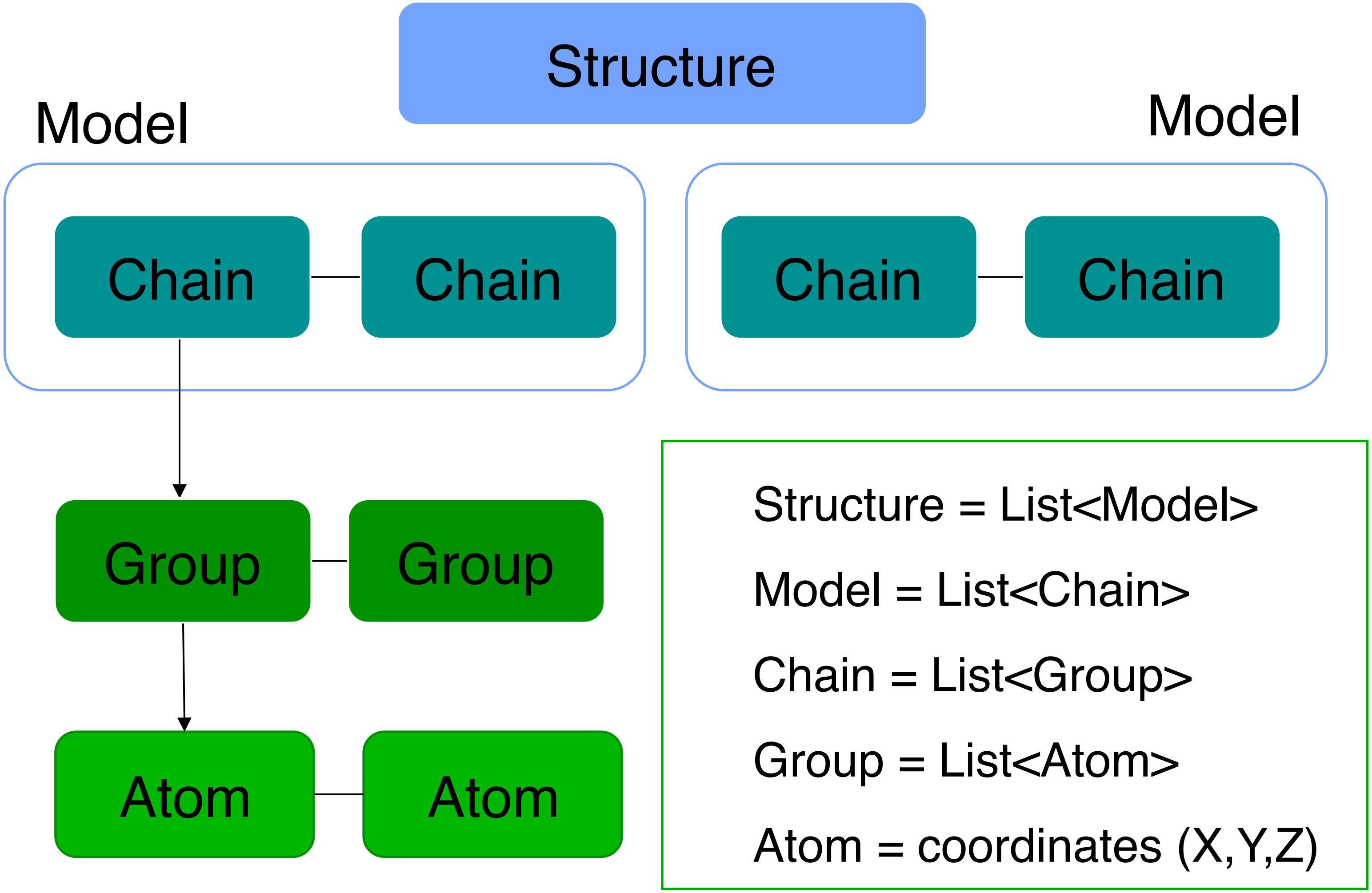
PART 2
BioJava Structures

Structure objects

Loading and writing

Operations

Structure Objects



Structure = List<Model>

Model = List<Chain>

Chain = List<Group>

Group = List<Atom>

Atom = coordinates (X,Y,Z)

Group Types

- **BioJava** uses the **Chemical Component Dictionary** to assign group types
  - Amino Acid (L-peptides)
  - Nucleotide (DNA or RNA)
  - Waters
  - Hetatoms

https://github.com/biojava/biojava-tutorial/blob/master/structure/chemcomp.md

Loading Structure Objects

- **AtomCache**
  - PDB ids (2HHB)
  - Structural ranges (2HHB.A:1-20)
  - SCOP, CATH & ECOD ids (d2hhba_)
  - Many configuration options

- **StructureIO**

Demo 2

- Load a structure in different formats
- Write a structure from BioJava to a file

Problem 2

- **Traverse BioJava structures**
  - **Task 1**: number of models. Hint: *nrModels*
  - **Task 2**: number of polymer chains. Hint: *PolyChains*
  - **Task 3**: number of amino acids in a chain.
    - Take a look at the *GroupType* class first
    - Hint: use one method from the Chain object
  - **Task 4**: number of oxygens in the amino acids of a chain.
    - Take a look at the *Element* class
    - Hint: use a double loop iteration over List of Groups and Atoms

PART 3
BioJava Applications

Biological assemblies

Visualization in Jmol

Biological Assemblies

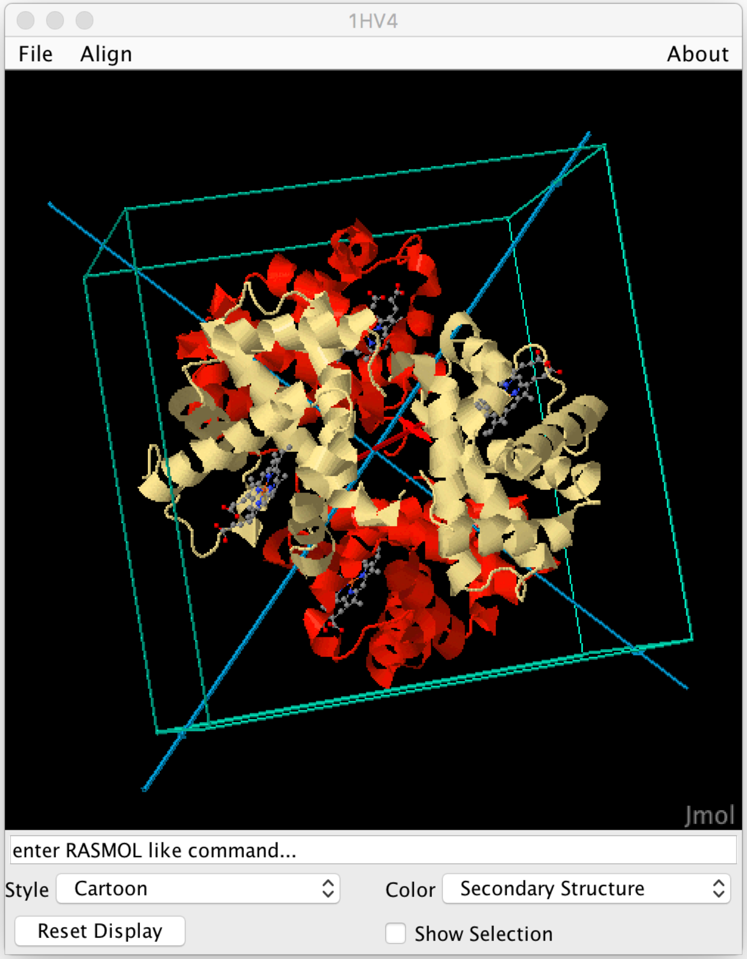
- **Important concepts**
  - Asymmetric Unit (AU)
  - Unit cell
  - Crystal lattice

- **Resource:**
  - https://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/biological-assemblies

Visualization in Jmol

- Interface for **quick** and **simple** visualization of structures in **Jmol**

1. Start a **JFrame**
2. Insert a **Jmol** panel
3. Convert the **BioJava** structure to a structure file (PDB, MMTF)
4. Send the structure file to the **Jmol** panel



enter RASMOL like command...

Style: Cartoon

Color: Secondary Structure

□ Show Selection

Problem 3

- **Display the symmetry of a biological assembly**
  - **Task 1**: download a biological assembly.
    - Hint: use the StructureIO class directly.
    - Warning: set the multiModel option to true (false is default) to be able to visualize the results (due to limitation of single letter chains in PDB format)
  - **Task 2**: change the parameters for pseudo-symmetry analysis.
    - Hint: structural clustering instead of sequence.
  - **Task 3**: obtain the symmetry and stoichiometry from the result.
    - Hint: use getter methods.

Contributing

- Do you want to use BioJava for your project?
- Do you have any ideas?
- Would you like to stay tuned?

- Join us at:
  - GitHub issues: https://github.com/biojava/biojava/issues
  - Mailing list: http://biojava.org/wiki/BioJava%3AMailingLists
  - Gitter: https://gitter.im/biojava/biojava

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