Web Lab 2 – architecture overview

Jonathan Cooper, UCL

Web Lab 2 Architecture

- Ansible deployment of entire stack
- Including local developer version

Developing the user interface

- Live demos
    - WL1: https://chaste.cs.ox.ac.uk/WebLab
    - WL "1.5": https://muck.cs.ox.ac.uk/FunctionalCuration & https://lofty.cs.ox.ac.uk/FunctionalCuration
   - WL2: https://scrambler.cs.ox.ac.uk

Representing information
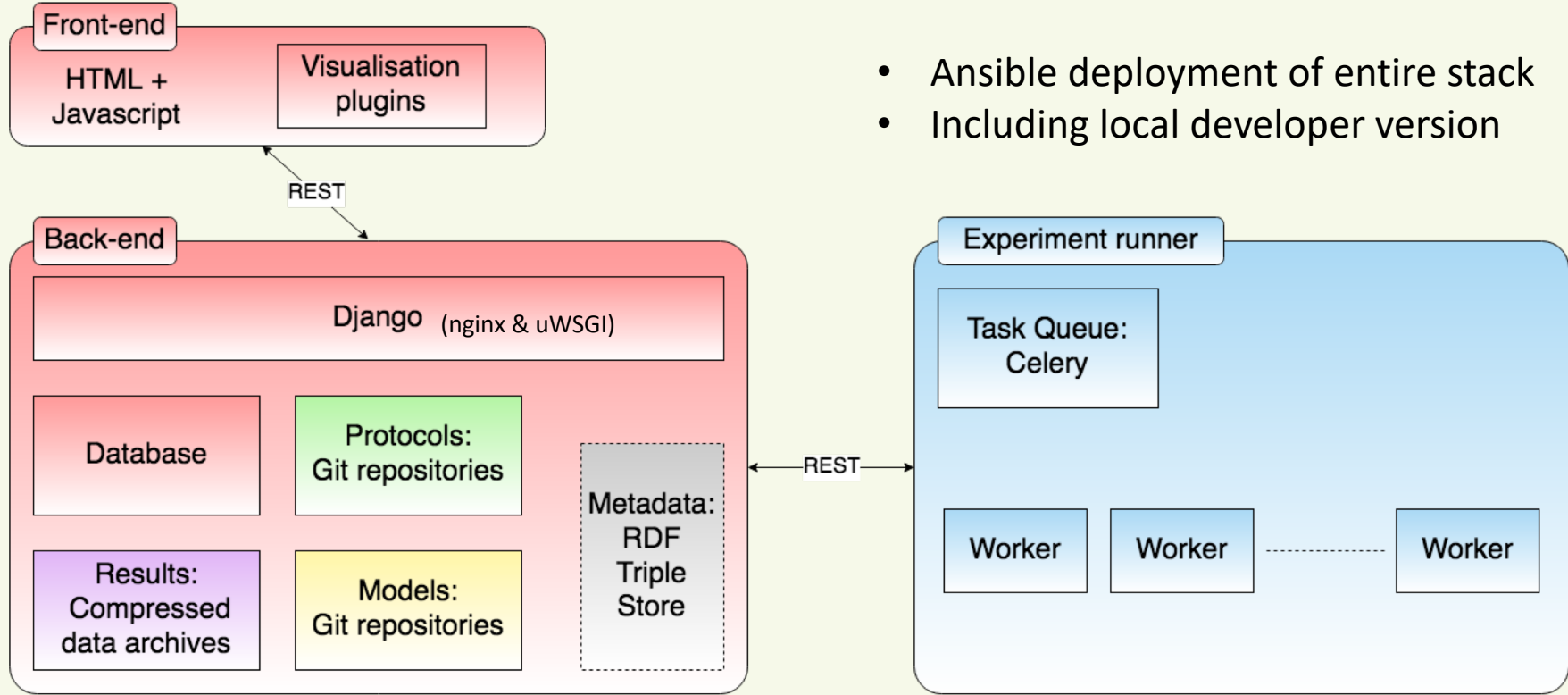
- How do we represent models, protocols, data, fitting specifications, results, … so as to
  - Exploit commonalities?
  - Make them useful to other tools / researchers?
  - Easily import from other sources?
  - Make connections and find information?

Representing information

- Models and protocols: version controlled repositories, with OMEX manifest

- Fitting specification: a type of protocol?
  - Can it be applied to any model?
  - Has more inputs: model, protocol and ref data
  - Results include parameter distributions

- Data: file formats?

Manipulating CellML models

Asif Tamuri, UCL

Conceptual overview
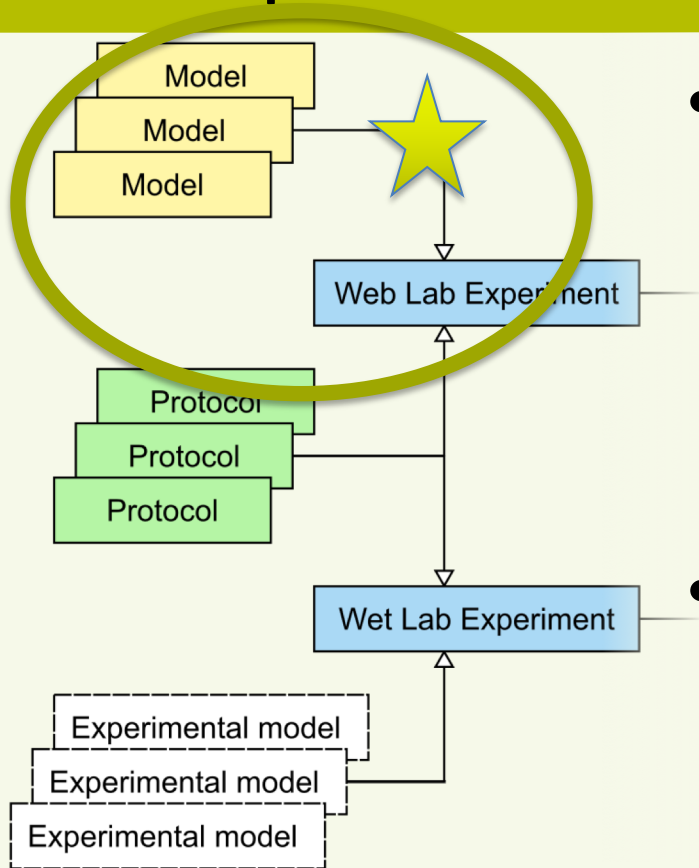
- CellML format describes model
  - ODE system of cardiac cells
  - Equations in MathML
  - Variables, Connections, Units, Metadata

- Environment to manipulate the model
  - Prepare for solving

cellmlmanip library

- Overlaps with PyCML

- Translate CellML maths
  - Sympy equations

- Annotate/manipulate equations

```
<math><apply><eq/><apply><diff/><bvar><ci>t
ime</ci></bvar><ci>m</ci></apply><apply><mi
nus/><apply><times/><ci>alpha_m</ci><apply>
<minus/><cn cellml:units="dimensionless">
1</cn><ci>m</ci></apply></apply><apply><tim
es/><ci>beta_m</ci><ci>m</ci></apply></appl
y></apply></math>
```

```
Eq(Derivative(m(time), time),
    alpha_m*(-m + 1.0) - beta_m*m)
```

```
Eq(Derivative(m(time), time) * dimensionless/millisecond,
    alpha_m/millisecond * (-m*dimensionless + 1.0*dimensionless) -
    beta_m/millisecond * m*dimensionless)
```

Possible discussions/work

- Tests for mathml2sympy transpiler
  - Multiple equalities, Sympy Symbol equality, interesting/difficult maths

- Unit handling
  - Quirks of Sympy unit handling
  - Conversion/simplification/checking
  - …alternatives?!

Annotations in Web Lab 1

- RDF embedded within CellML files
- "Oxmeta" ontology from the Chaste project
  - Just the terms we've needed for electrophysiology
- Protocols reference these URIs
  - E.g. `oxmeta:membrane_voltage`
  - List of optional/required URIs stored in DB
- Javascript drag & drop annotation tool for models

Future annotation directions

- Improvements in organising annotations
  - Separate annotation files in repositories
  - Which predicates to use
- Use of community-agreed ontologies
- Search & (more) reasoning
  - Facilitated by triple store

Goals for the Web Lab Workshop

Discussion

What are the key issues around building mathematical models of biology from experimental data?

Key issues

Workshop working groups

- Roadmap / white paper publication
- Specifying & running experiments
- Inference tools & fitting experiments
- CellML handling & model manipulation
- Repository interfaces (and data stores)
- Annotation & ontologies
- User interface design & information architecture