temporal logic

- `is-jetlagged(Joe)`
- `doesnt-want(to-bore-you, Joe)`
- `concerned(Joe)`
- `may-need(Joe, periodic-reminder)`

Data Sharing in Laboratory Science

towards a Protégé solution

Joe Edelman
formerly: fMRI Data Center (NIH/NSF)
still: Dartmouth College

Overview

- the problem of scientific data management
- our approach to it: data model & interfaces
- current status of the project

Scientists want...

- to understand & reanalyze data from outside their discipline
- to analyze someone else's data as easy as their own
- to apply new analysis techniques to large quantities of old data automatically
- to use model-agnostic techniques (clustering, etc) to mine and to relate new raw data to older data

But...

they can't have it

- different data/knowledge exchange for lab-local and interlab use
  - **lab local**: C-structure binary files, columnar text files, spreadsheets, and form-based systems like Matlab's GUI, MS Access, and FileMaker Pro
  - **interlab**: journal articles, figures, and a variety of semi-structured networked results databases (Genbank, ACEDB, PDB, etc).
- (re)analysis can only be done lab-locally or by special request

So...

Layered Solution

- make a core semantic data model for laboratory science
- deploy tools that operate on this core for exchange of data & knowledge between fields
- extend this core for each domain or even each lab, to ease lab-local use
- work towards the ease-of-use and robustness of the best existing systems: files, forms, RDBMSes

But...

Challenges

- **bridging data & knowledge systems**
- **files are hard to beat**
  - easy to understand, organize, and integrate
- **FileMaker is hard to beat**
  - high data integrity, simple forms
- **extensibility can be messy**
  - reconciling parallel extensions
  - maintaining a useful core

Try anyway

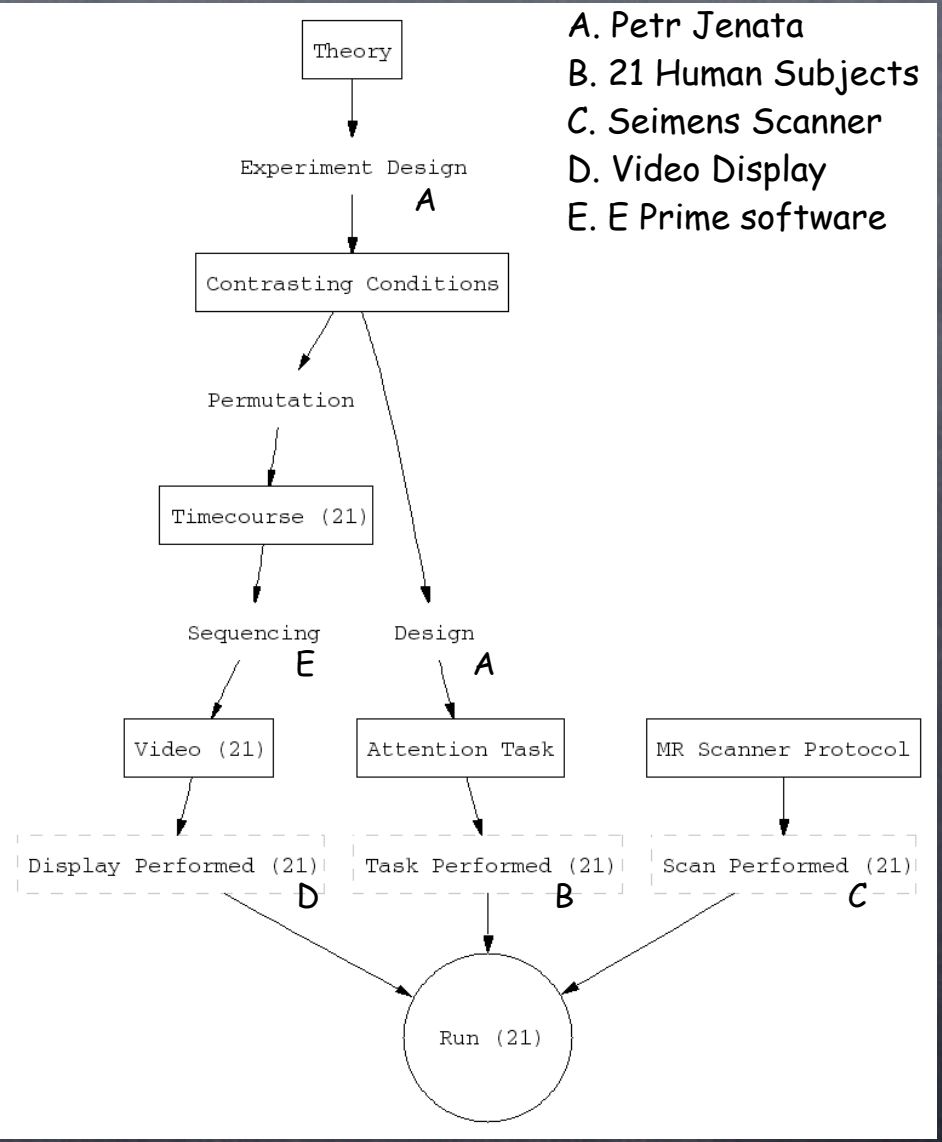
- tell you about the data model
- tell you about the interfaces
- review these challenges to see how well we've done

An eScience Ontology

Graphical Depiction

(a key advantage)

- input-to, output-from, DIRECT-TYPE, consists-of, performed-by
- Using just these core relations, we can display a graphical *interdisciplinary summary* of the experiment.
- scientists have been very positive about this summary in interviews



Graphical Depiction

(a key advantage)

- input-to, output-from, DIRECT-TYPE, consists-of, performed-by, model
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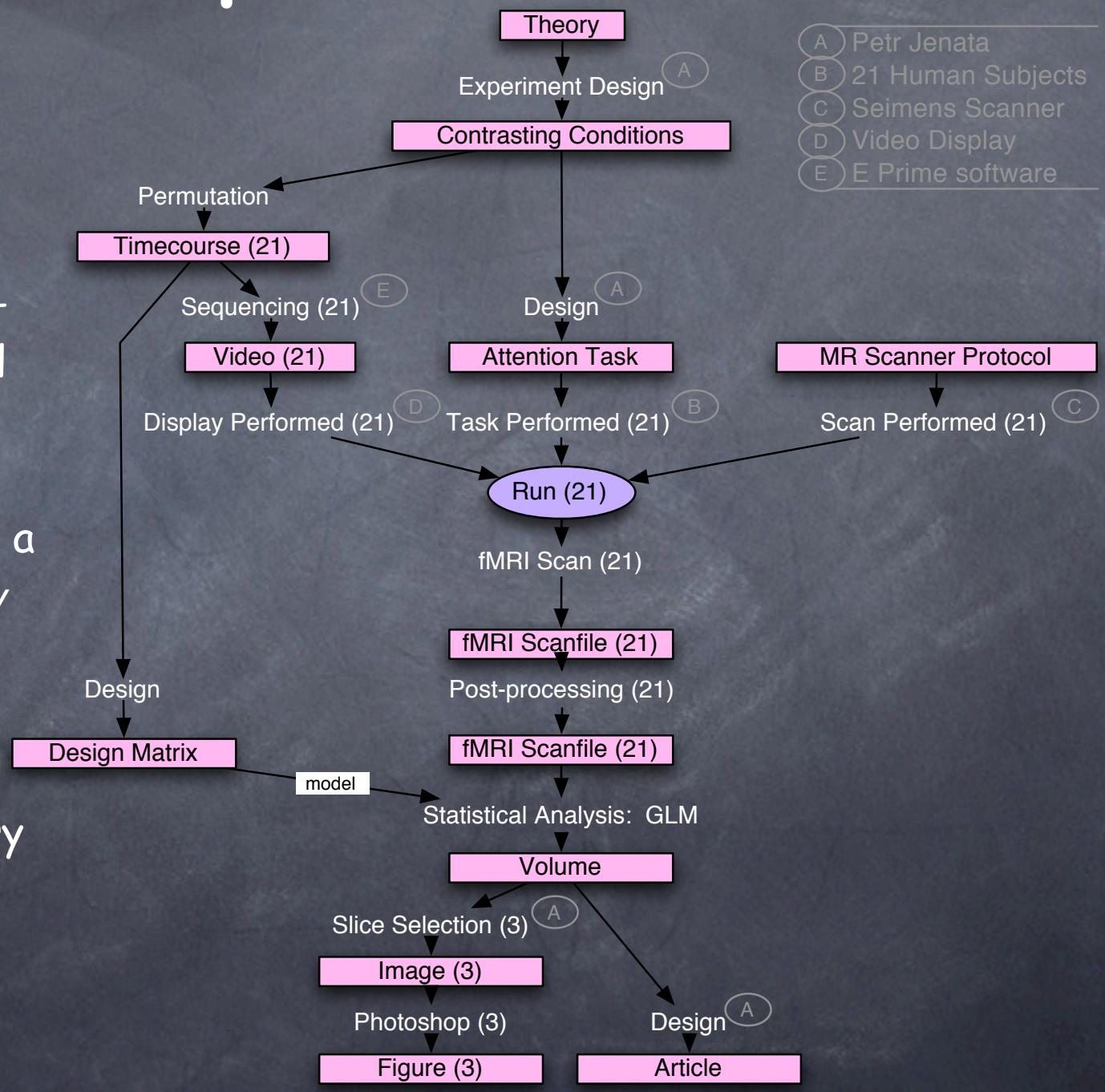
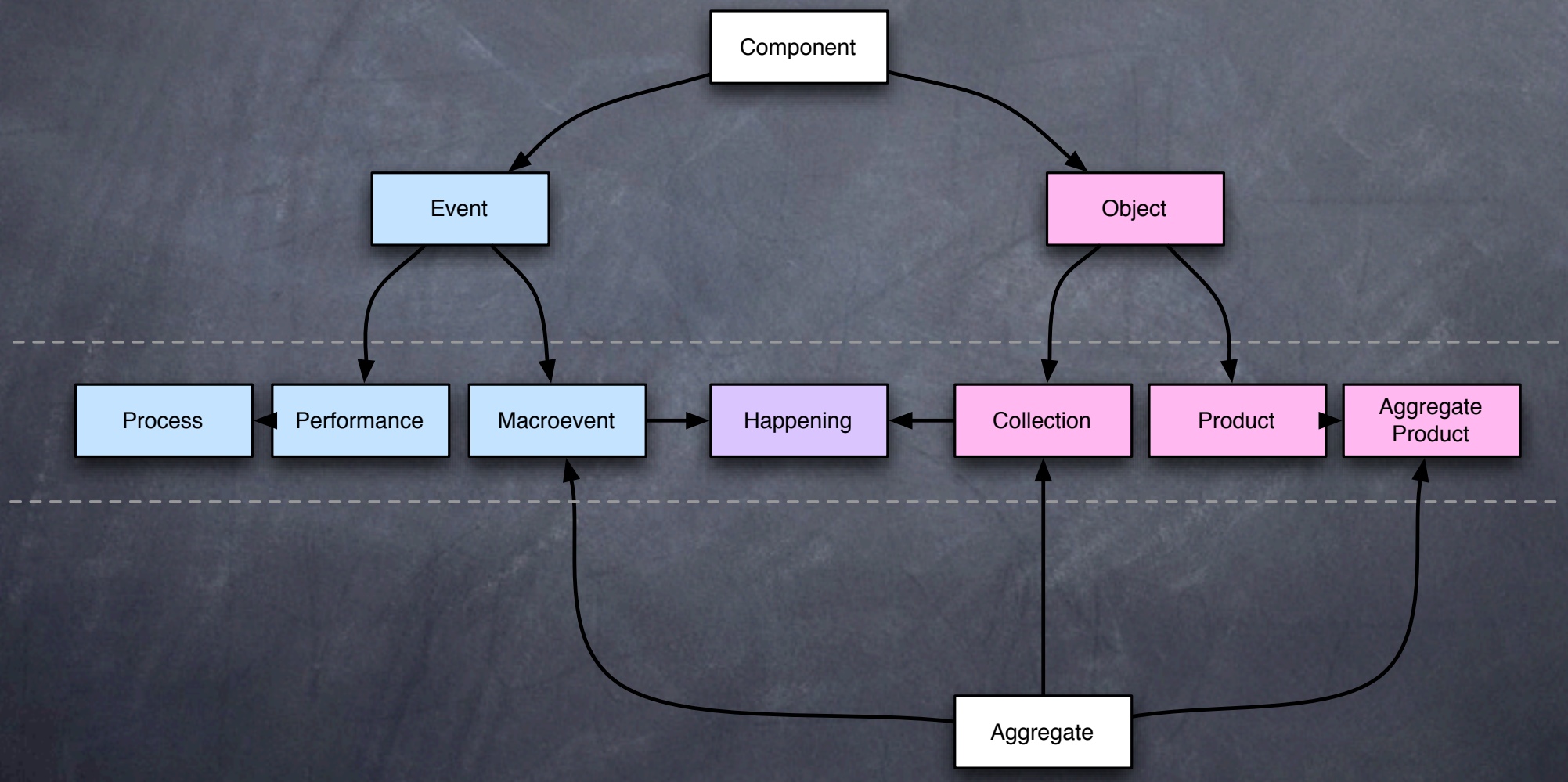
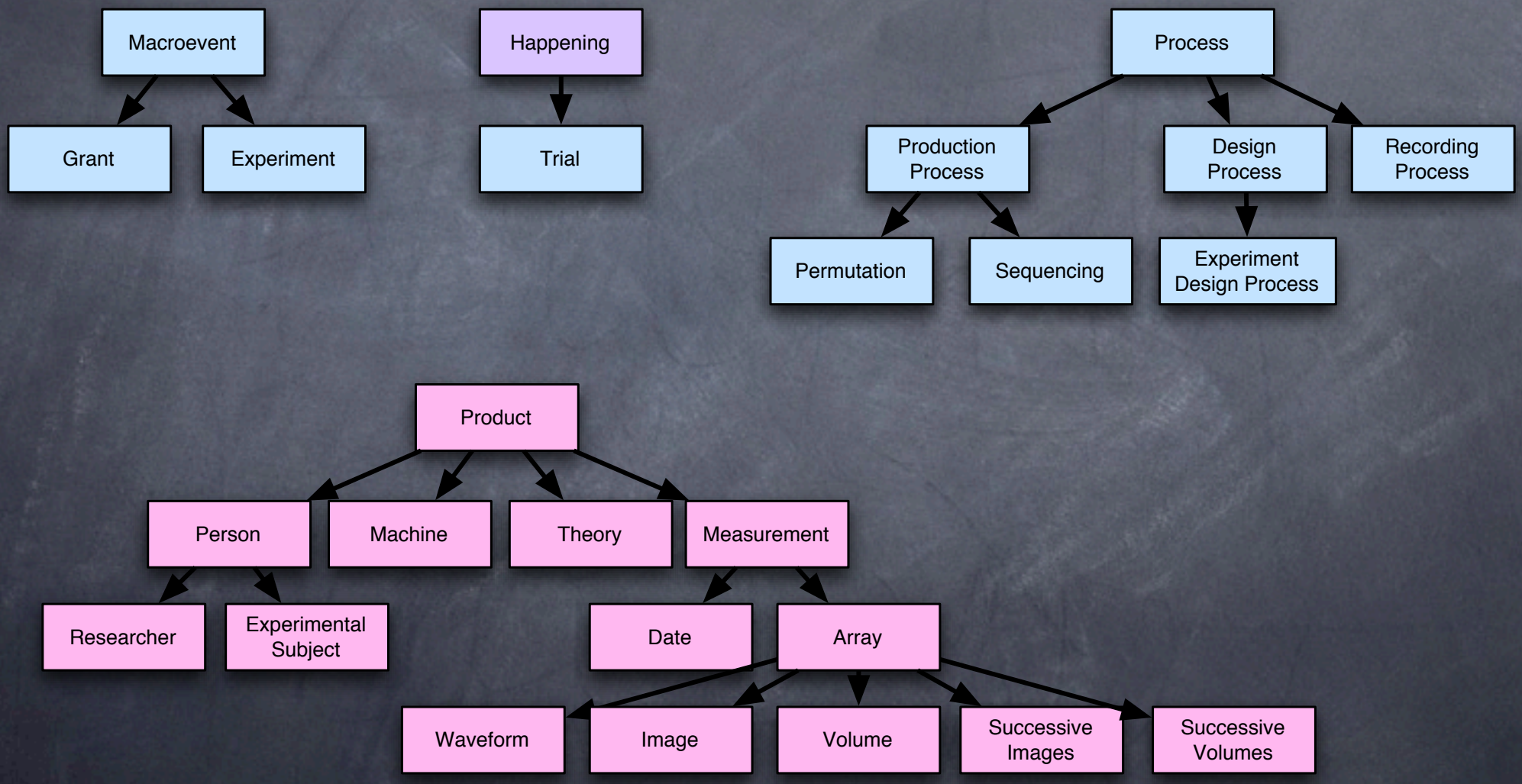


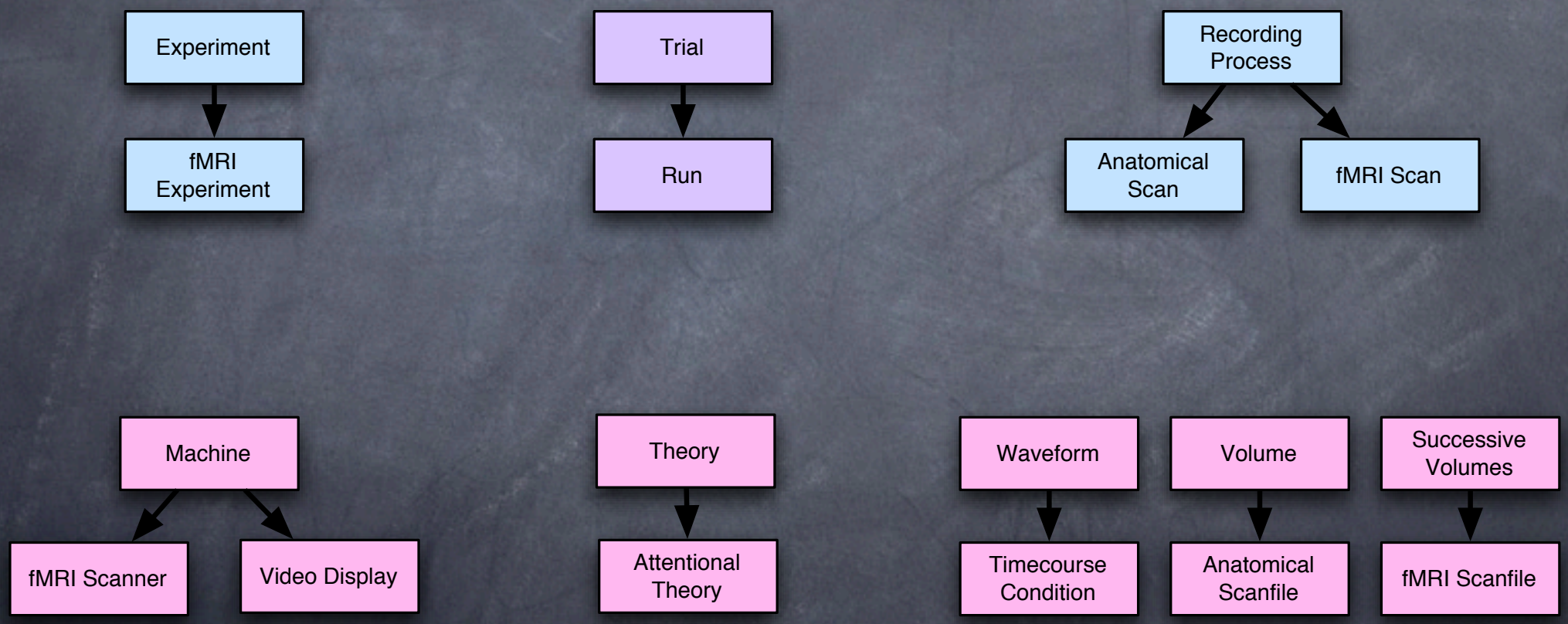
Product / Process Data Model



Experimental Design, Setup, Recording, and Analysis Ontology (EDSRA)



EDSRA-fMRI


Experiment
fMRI Experiment
Trial
Run
Recording Process
Anatomical Scan
fMRI Scan
Machine
fMRI Scanner
Video Display
Theory
Attentional Theory
Waveform
Timecourse Condition
Volume
Anatomical Scanfile
Successive Volumes
fMRI Scanfile

EDSRA - Queries

- **measurement / recording**
  - what is being recorded?
  - what device was used to make the measurement?
  - is this measurement continuous or discrete?
  - etc
- **analysis**
  - has this data been normalized, filtered, etc?
  - what analyses are available? which possible analyses apply?
  - can this analysis be reproduced exactly from its antecedents?
  - etc

EDSRA - Decompositions

- as various experiments
- as various kinds of objects about which data has been collected (human subjects, tasks, scanners)
- as measurements, volumes, waveforms, etc.
- as tested mathematical models and theories

Method of Extension

- facet overrides used extensively
- keeps all information accessible using core model
- provides for domain specific guidance in data entry

Name: Scan Performed
Documentation:
Constraints:
Role: Concrete

Template Slots

Name	Type	Cardinality	Other Facets
S performed-by	Instance	required single	classes={fMRI Scanner}
S input I	Instance	required single	classes={MR Scanner Protocol}
S part-of I	Instance	multiple	classes={Happening}

Name: MR Imaging
Documentation:
Constraints:
Role: Concrete

Template Slots

Name	Type	Cardinality	Other Facets
S output I	Instance	required single	classes={Anatomical MRI Scan}
S performed-by	Instance	single	classes={Object}
S input I	Instance	required single	classes={Run}
S part-of I	Instance	multiple	classes={Macroevent}

interfaces to the ontology

Advantages of Protégé

- preeminent tool for managing data in semantic data models
- cleanly designed in Java with easy extension in mind
- multiplatform, can be RDBMS or file backed
- guides data entry / knowledge acquisition intelligently using ontology
- can be queried in many ways by using different tabs
- thriving community

lacking in Protégé

capability

- support for large multihomed files
- support for measurements, arrays, mathematical functions, etc

usability

- simple hierarchical and graphical methods of browsing (comparable to those for filesystems)
- alternatives to KnowledgeBase API java for getting data in and out programmatically
- support for derived data / views / normalization

our extensions

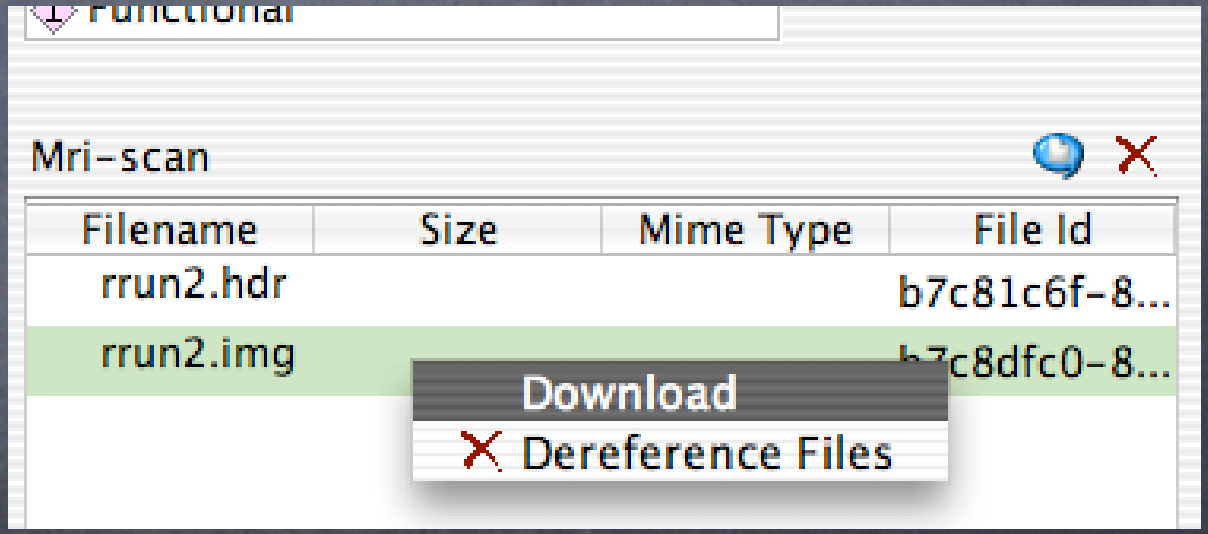
- support for large multihomed files
- support for measurements, arrays, mathematical functions, etc
- simple hierarchical and graphical methods of browsing (comparable to those for filesystems)
- alternatives to KnowledgeBase API java for getting data in and out programmatically
- support for derived data (and normalization)

Coming this fall

support for large multihomed files

work by Jeff Woodward

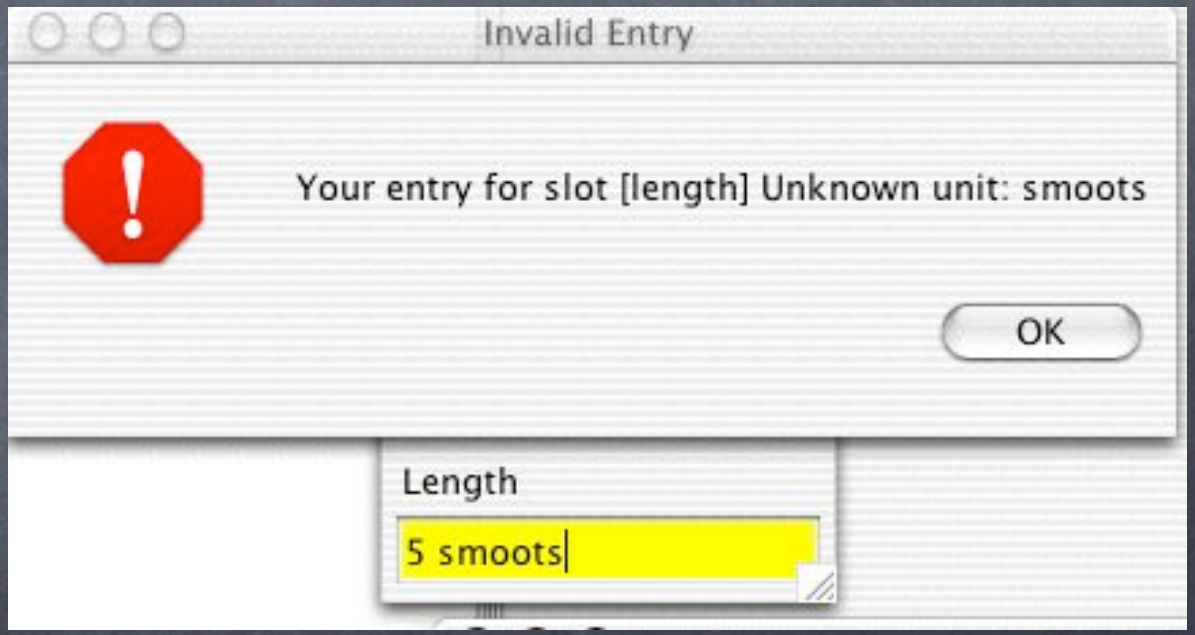
- UUIDs / surrogates
- checked against multiple file resolvers
- resolved to URLs
- good with NFS, AFS, HTTPS, etc
- "tfile://" prefix supports removable media



support for measurements, arrays, mathematical functions

with Jeff Woodward

- **units of measure**: attribute of "float" scalar and compound (recording, image, volume) types
- **quantity**: ontology and data entry support, no query support
- **1D, 3D, and 4D visualization**



support for measurements, arrays, mathematical functions

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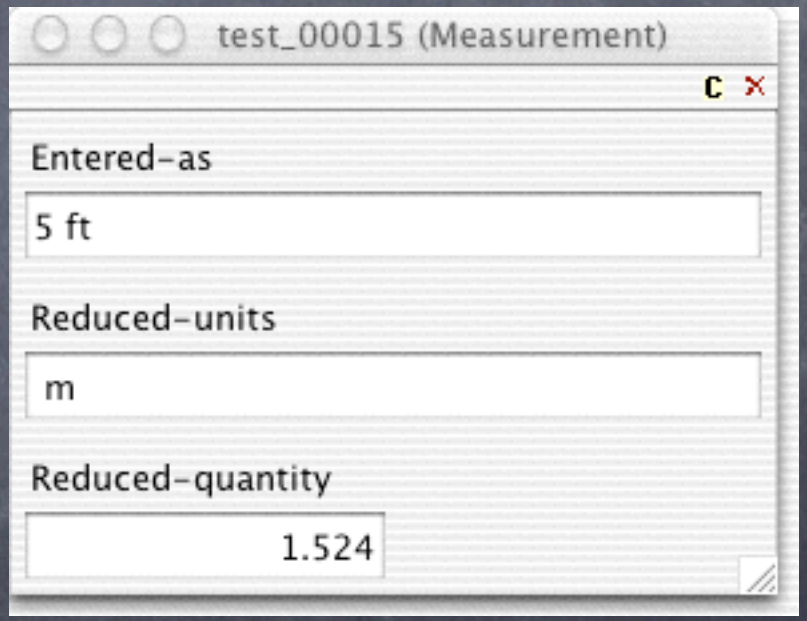

support for measurements, arrays, mathematical functions

work by Bennet Vance

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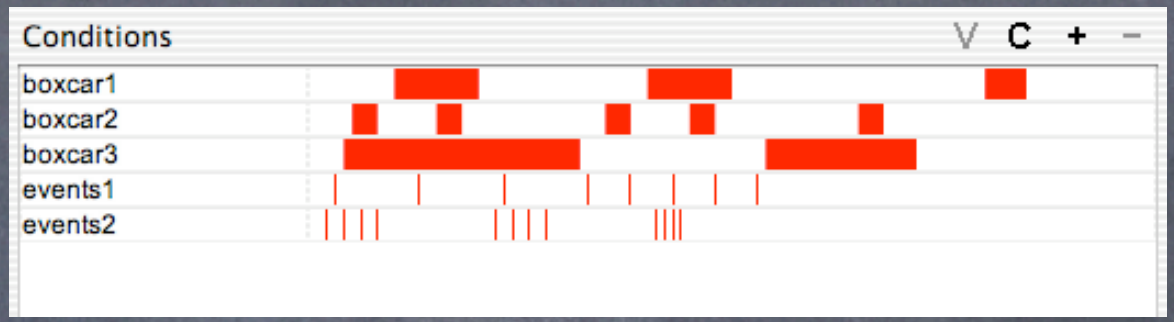
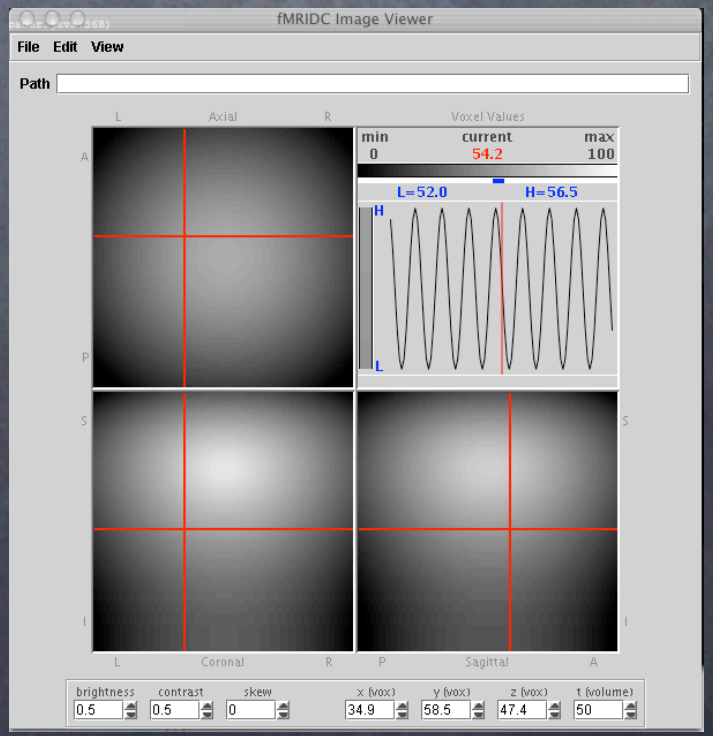
- **1D, 3D, and 4D visualization**





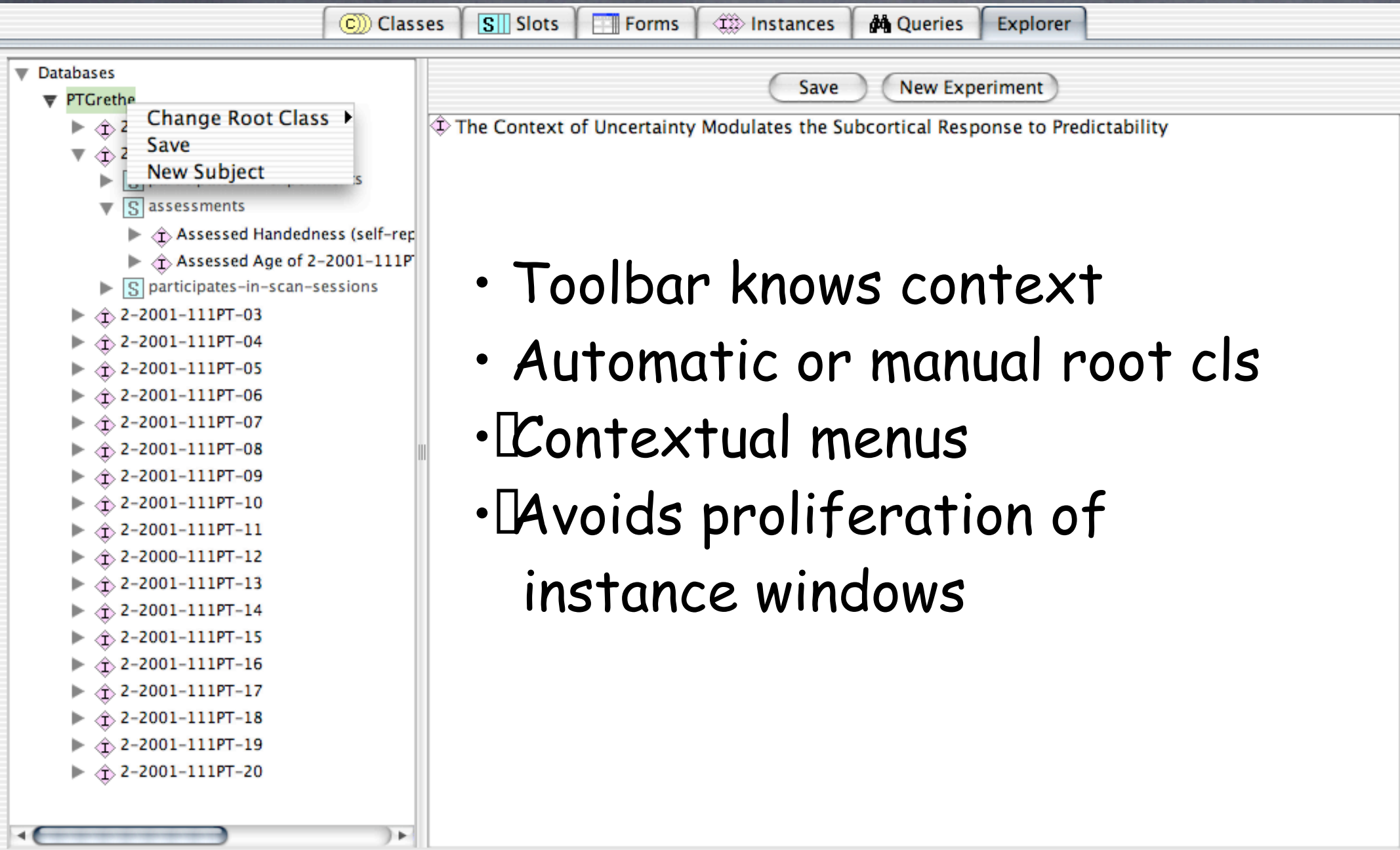
simple hierarchical and graphical methods of browsing

(comparable to those for filesystems)

- **ontology-neutral**
  - knowledge explorer
  - browser formats
  -
  - coalescing graph widget

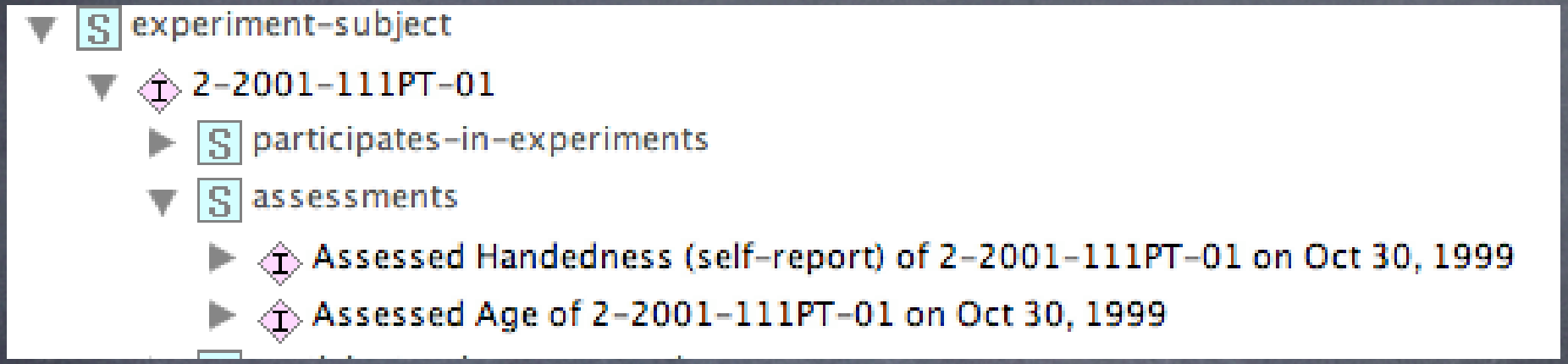
Coming this fall

Explorer Tab



- Toolbar knows context
- Automatic or manual root cls
- Contextual menus
- Avoids proliferation of instance windows

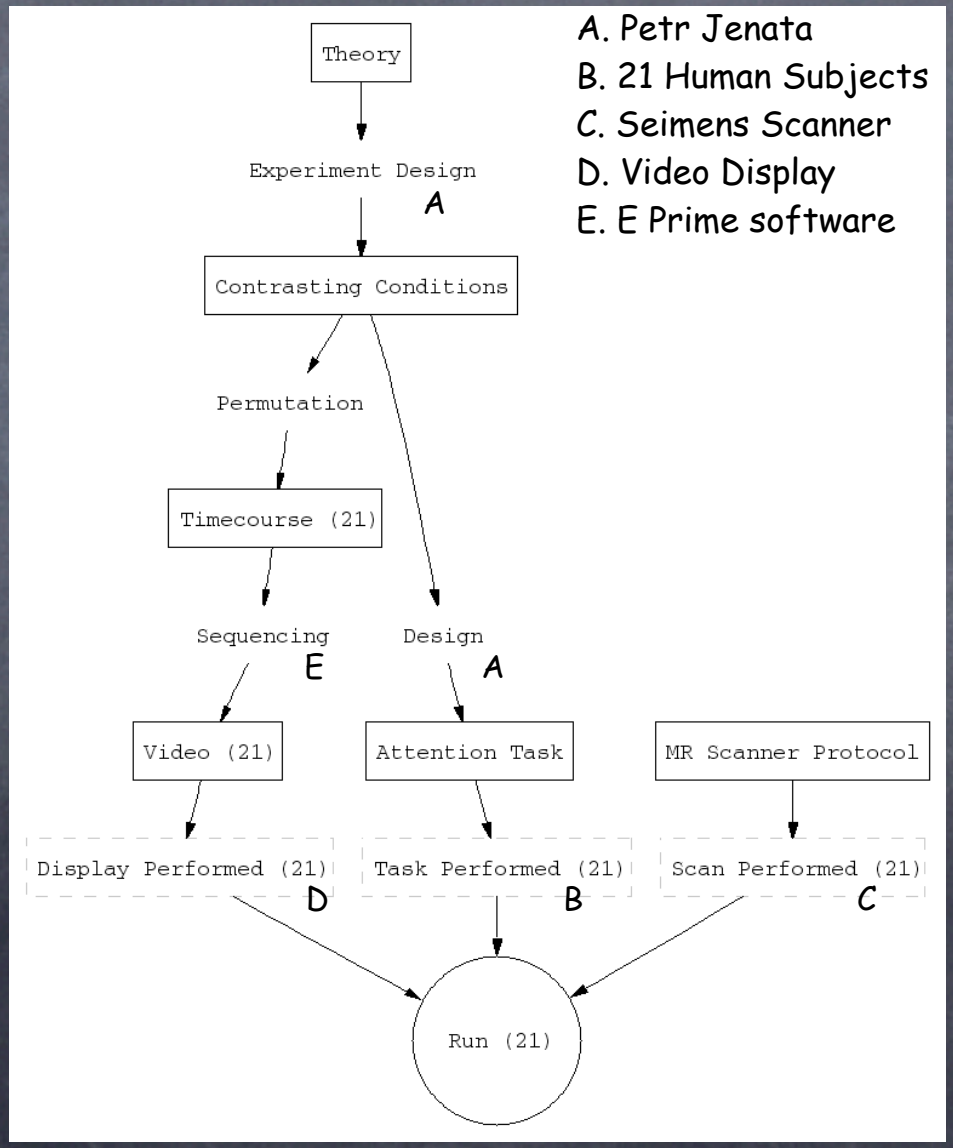
Browser Formats




```
s = "Assessed ${:DIRECT-TYPE}”
  + “ of ${assessment-subject}”
  + “ on ${start-date}";

project.setDirectBrowserFormat(assessmentCls, s);
```

Coalescing Graph Widget



alternatives to KB API for programmatic data access

- **Two simpler syntaxes:**
  - Simple Java API
  - Component Paths

```
listInstances("Dog")
.with("Owner", i);
```

```
dog.list("owners")
.makeWith("name", "Jim");
```

- Perl, Python, & Unix command line bindings

Coming Soon

- FormWidget Actions

alternatives to KB API for programmatic data access

- **Two simpler syntaxes:**
  - Simple Java Queries
  - Component Paths

    "/NSF2003/Motion/Scan:jxe-sep28-1/output"
- Perl, Python, & Unix command line bindings

Coming Soon

- FormWidget Actions

alternatives to KB API for programmatic data access

- **Two simpler syntaxes:**
  - Simple Java Queries
  - Component Paths

- Perl, Python, & Unix command line bindings

```
unix% wsrun http://fmridc.org/jws/daily/JavaServer.jnlp

unix% protege-add "/NSF2003/Motion/Scan:jxe-sep28-1/output" scan.img
```

support for derived data

- this fall
- solves problems with reified relations by making them appear as simple slots at the API level
- will allow viewing our KB as “just products” or “just processes”

Again...

Challenges

- **bridging data & knowledge systems**
- **files are hard to beat**
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- **FileMaker is hard to beat**
  - high data integrity, simple forms
- **extensibility can be messy**
  - reconciling parallel extensions
  - maintaining a useful core

current status of the project

- 50 neuroimaging experiments encoded using the ontology, available at http://fmridc.org
- 3 meta-analyses in the works
- deploying as lab-local data management solution at Berkeley, MIT, and Washington University Radiology Labs.

- future development of some features in some doubt
- all extensions open source and available
- preprint of ontology paper available soon

http://fmridc.org/dmt
http://sf.net/projects/fmri-dmt

jxe@dartmouth.edu

Availability

http://sourceforge.net/projects/fmri-dmt

Laboratory Features	files	/files
	measurements & dates	/widgets, /units
	1D viewer	/timecourse
	3D/4D viewer	/viewer, /image
User Interface	explorer tab	/ke
	browser formats	jxe@dartmouth.edu
	coalescing graph	12/2003
Programmatic Access	simple java api	/souffle/src/org/fmridc/protege/ProtegeUtilities.java
	pathname api	jxe@dartmouth.edu
	perl bindings	/souffle/scripts/putscan.pl
	unix bindings	/souffle/scripts/putscan.pl
	virtual slot framestore	12/2003
	python bindings	jnw@dartmouth.edu

Thanks!

- There is a long tradition of outstanding open source software developed by communities of academics:
  - Unix
  - Emacs
  - TCP / IP
- It takes skilled developers to make an extensible system.
- It takes an army to make a general purpose tool.