Predicting Workflow Performance

Hugo Hiden
Simon Woodman

e-science central

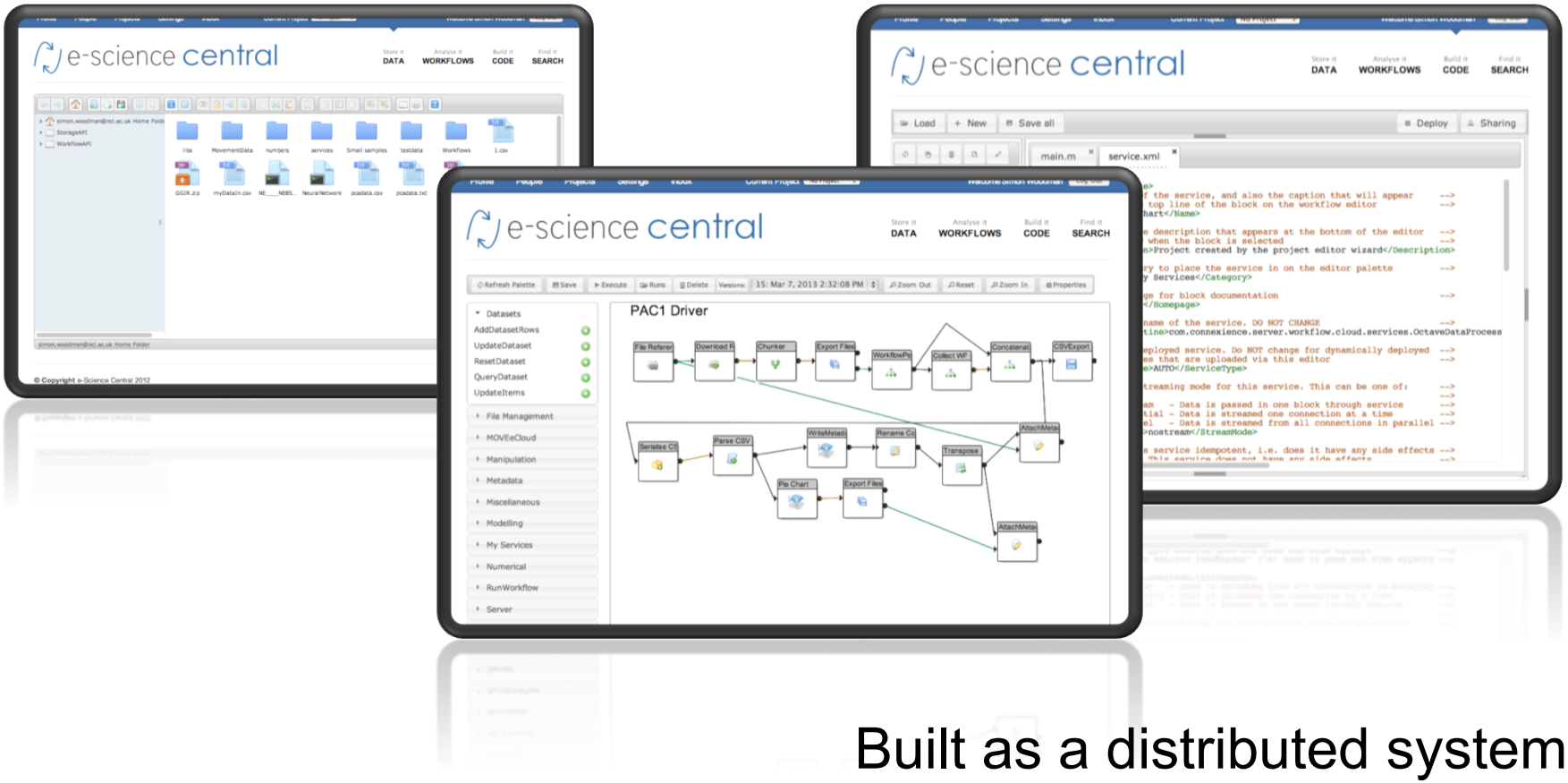
Newcastle University

Performance Prediction

- Good because:
  - Cost in Cloud
  - Know when to expect results
  - Capacity planning
  - Other work needs it
    - Paul's security
    - Scheduling
  - Other possibilities

e-Science Central

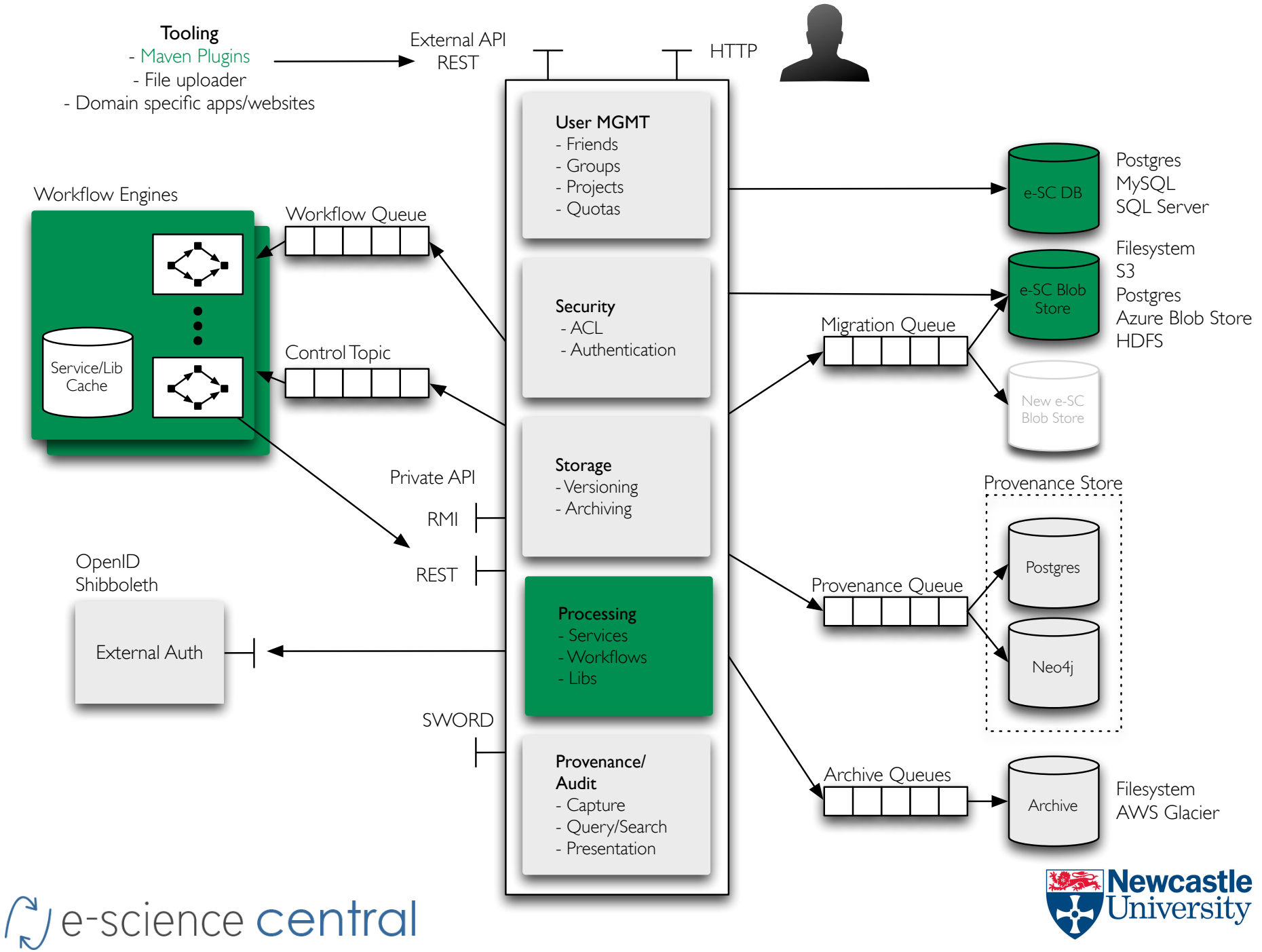
Platform for cloud based data analysis



Built as a distributed system…

e-science central

Newcastle University


Tooling
- Maven Plugins
- File uploader
- Domain specific apps/websites
External API
REST
HTTP
User MGMT
- Friends
- Groups
- Projects
- Quotas
Security
- ACL
- Authentication
Storage
- Versioning
- Archiving
Processing
- Services
- Workflows
- Libs
Provenance/
Audit
- Capture
- Query/Search
- Presentation
Workflow Engines
Service/Lib
Cache
Workflow Queue
Control Topic
Private API
RMI
REST
SWORD
OpenID
Shibboleth
External Auth
e-SC DB
Postgres
MySQL
SQL Server
e-SC Blob
Store
Filesystem
S3
Postgres
Azure Blob Store
HDFS
Migration Queue
New e-SC
Blob Store
Provenance Store
Postgres
Neo4j
Provenance Queue
Archive Queues
Archive
Filesystem
AWS Glacier
e-science central
Newcastle
University

Workflows for data processing

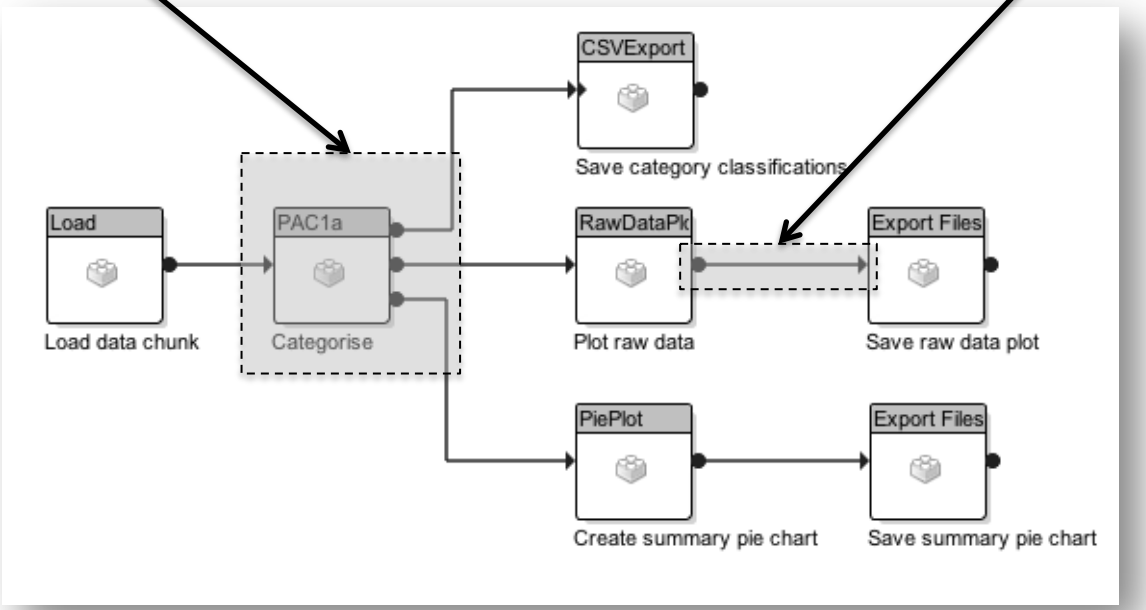
- Spreadsheets become unwieldy quickly
  - Emphasise data over process
  - Hard to see what has been done with data
    - Not obvious what calculations have been done
    - Hard to extract some of the the calculations and re-use them
  - Require everything to be done using the spreadsheets tools
    - May not include everything needed
- Workflows attempt to mitigate some of this
- Integrate different languages
  - Java, R, Octave, Javascript

Anatomy of a workflow

Workflows are made up of Blocks

Workflow block

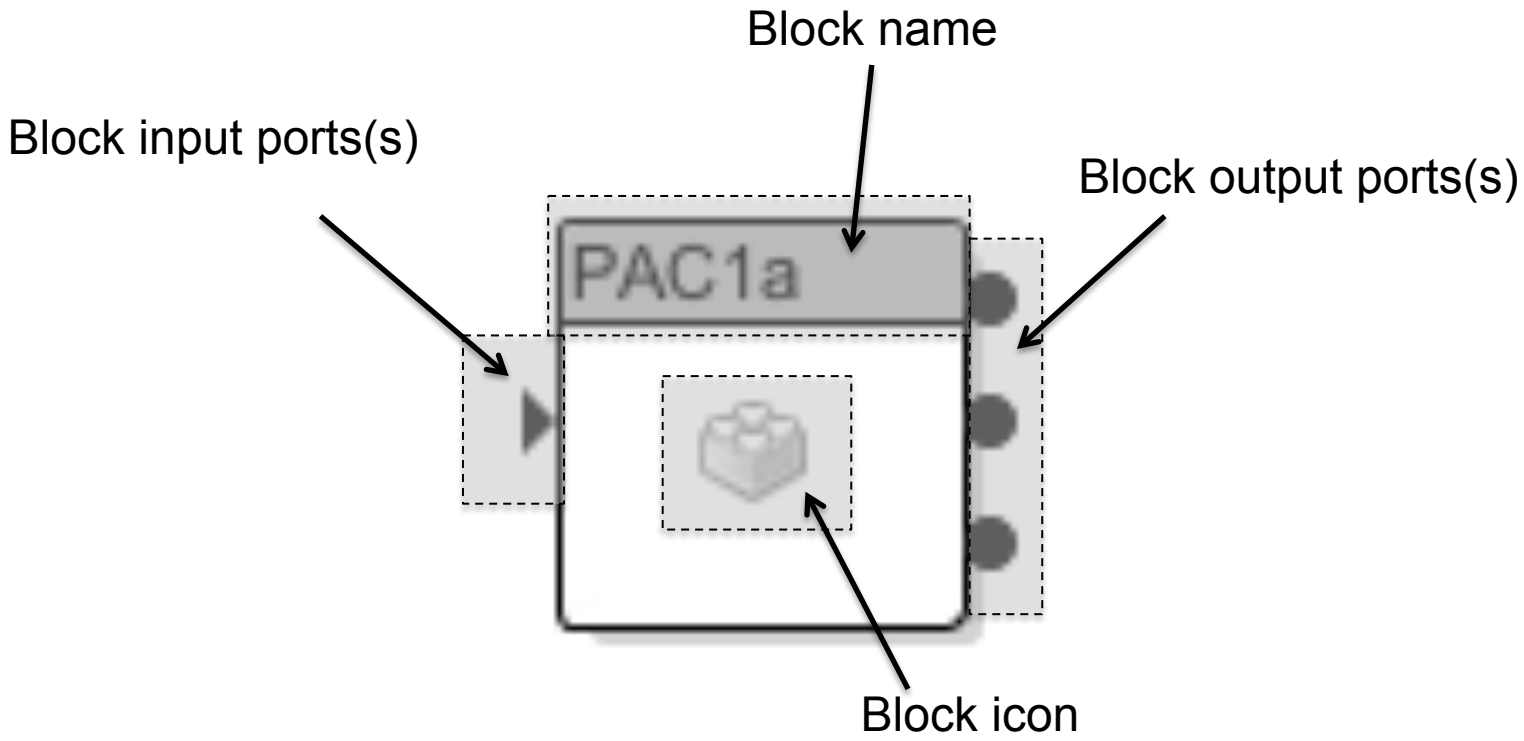
Data flows between Blocks in the direction of the arrows



e-science central

Newcastle University

Anatomy of a workflow Block

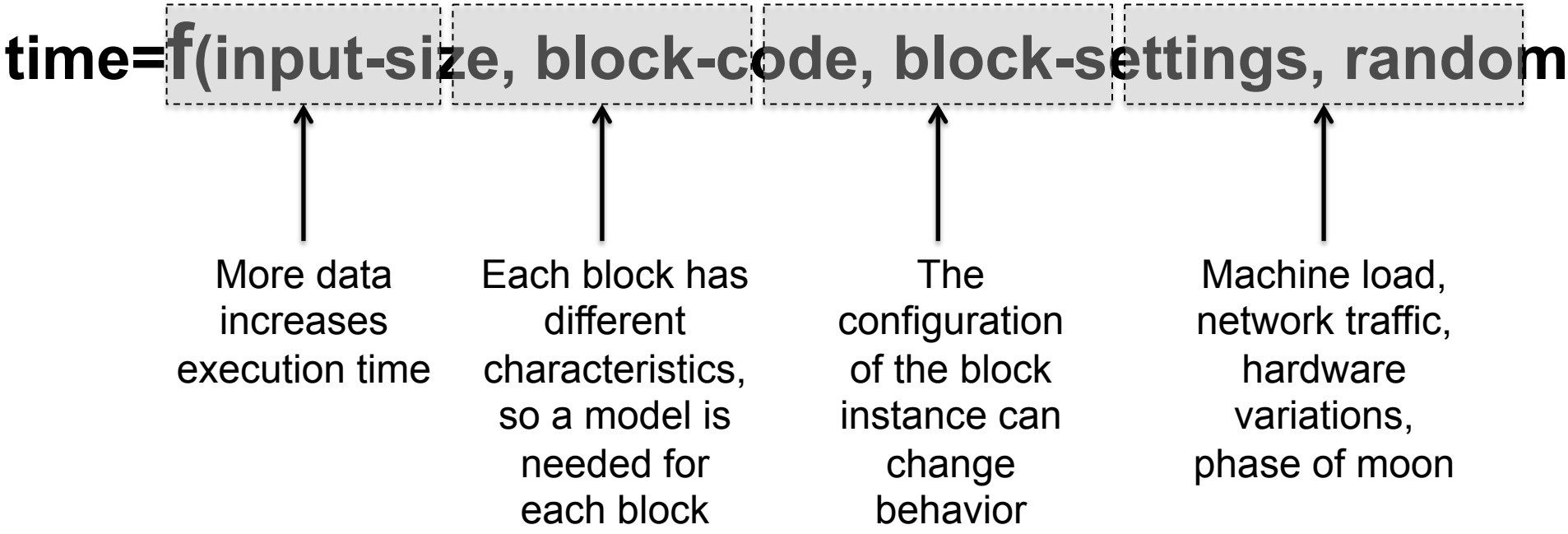


- Blocks read data from their input ports, process it and pass the results to their output ports
- Ports have specific meaning – e.g. on a block with multiple output ports, each port will typically contain a part of the result
- Each output port can be connected to multiple input ports on other blocks
- Only one connection is allowed per input port

Factors influencing performance

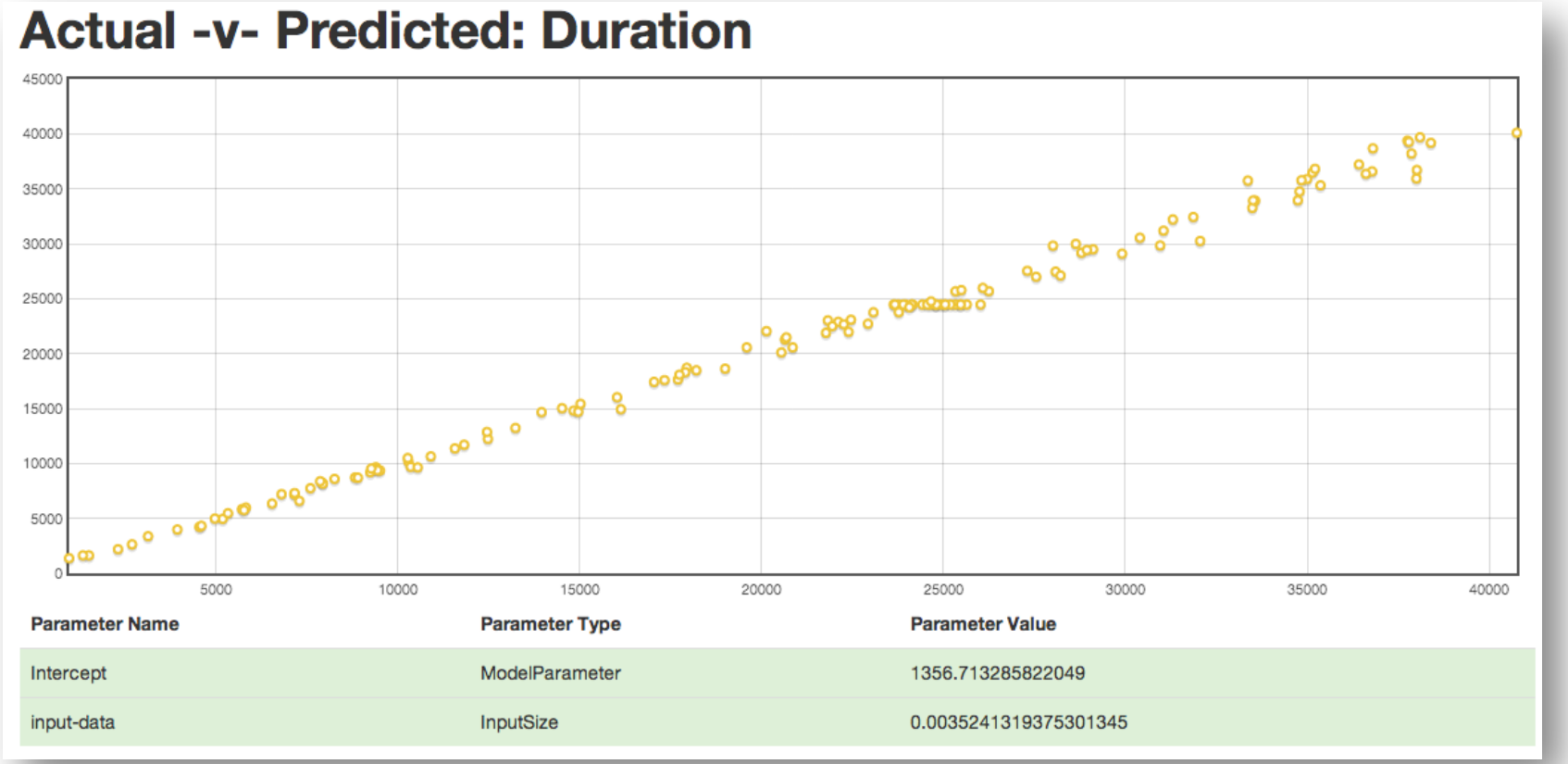
- Variable execution time
  - dedicated machine < local server < cloud VM
- There are good predictors
  - The code itself
  - The configuration of the block
  - The input data sizes
  - The machine it is running on
- Predictable?

Execution time of a block



A workflow is a connected pathway of blocks…

A predictable block

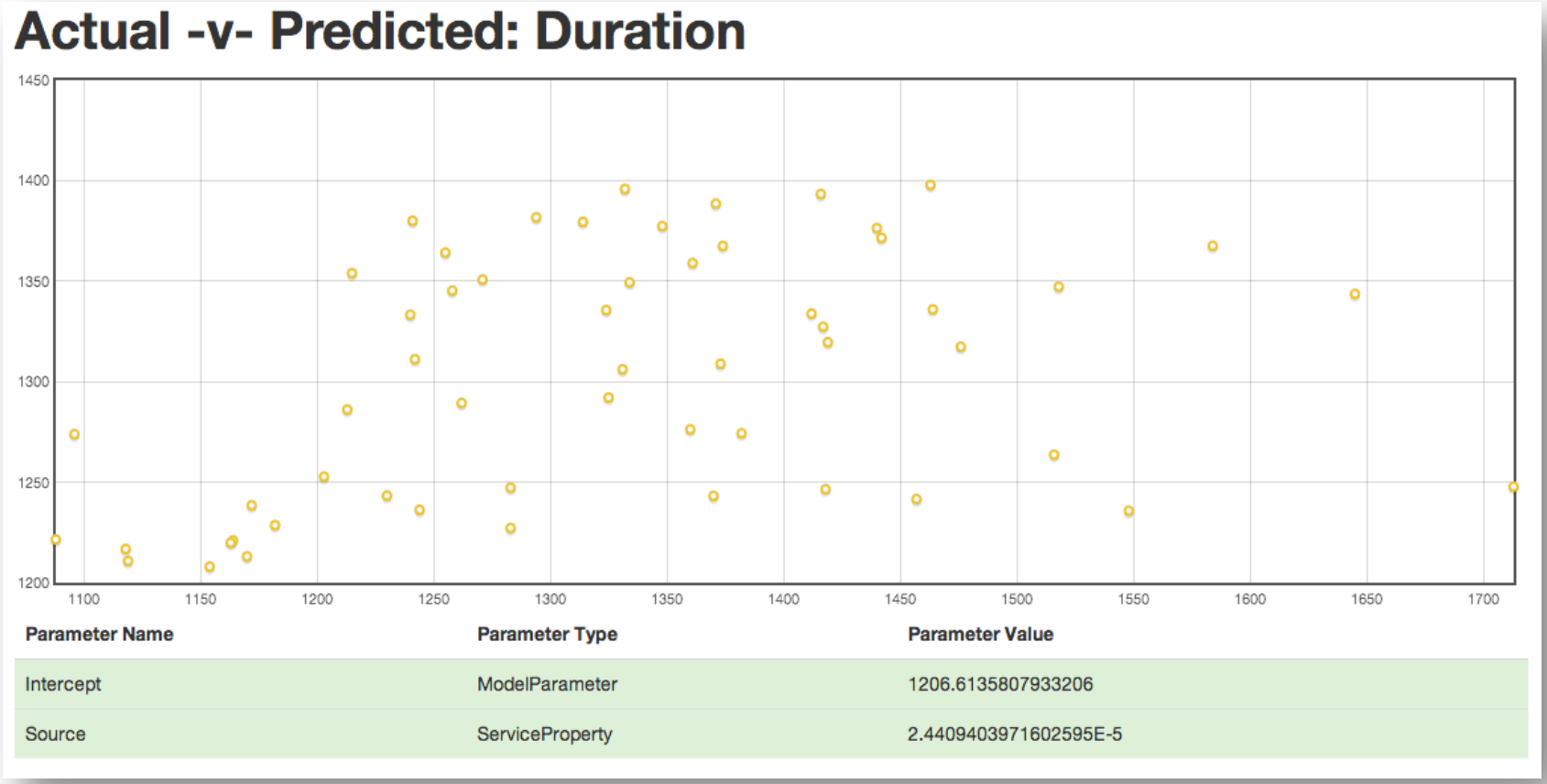


Parameter Name	Parameter Type	Parameter Value
Intercept	ModelParameter	1356.713285822049
input-data	InputSize	0.0035241319375301345

e-science central

Newcastle University

A less predictable block



Parameter Name	Parameter Type	Parameter Value
Intercept	ModelParameter	1206.6135807933206
Source	ServiceProperty	2.4409403971602595E-5

e-science central

Newcastle University

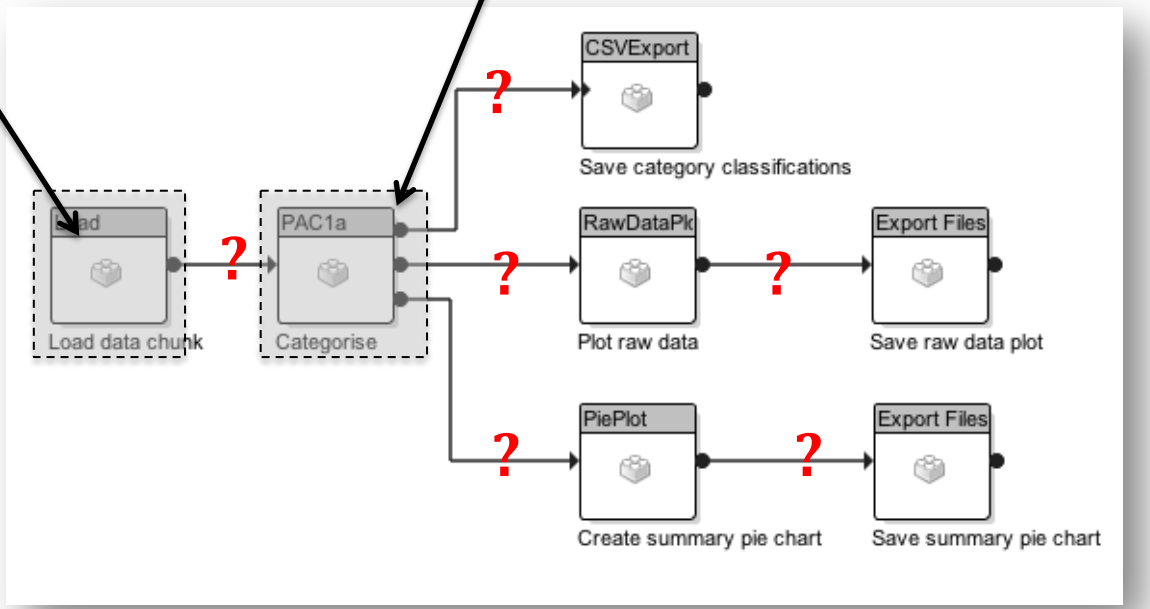
Predicting Workflow duration

Modelling is complicated by connected nature of workflow

All data for model readily available…

… not the case here

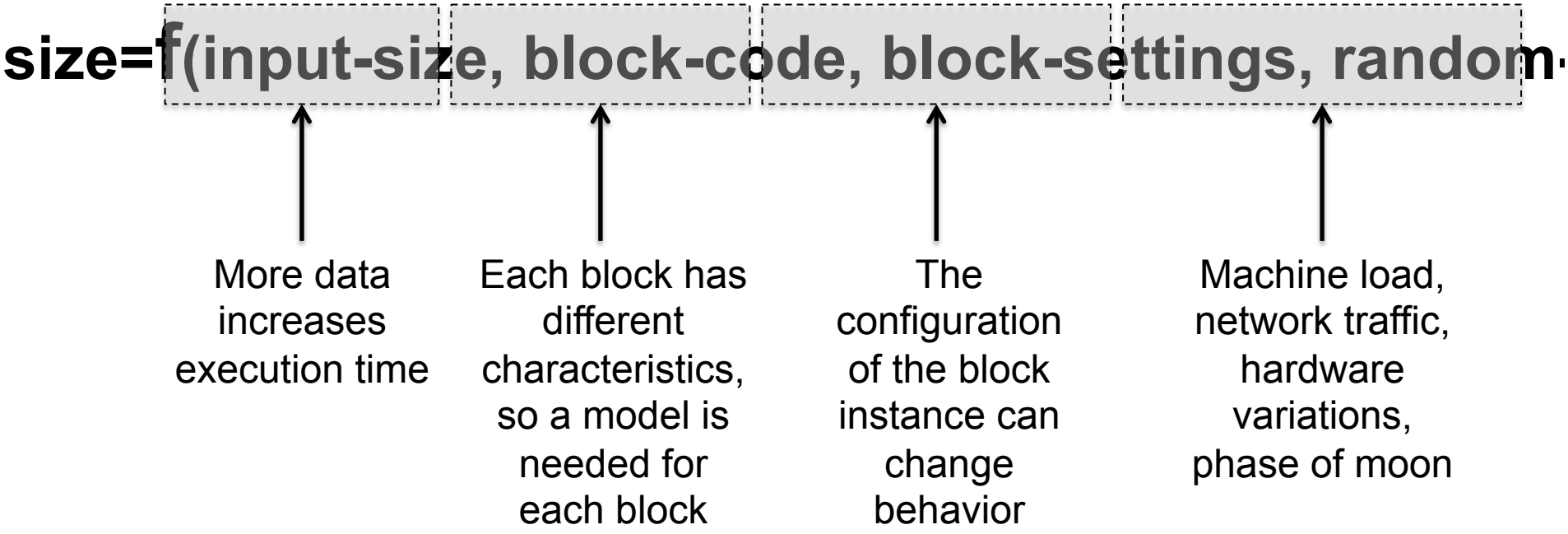
? how big are the intermediate data transfers



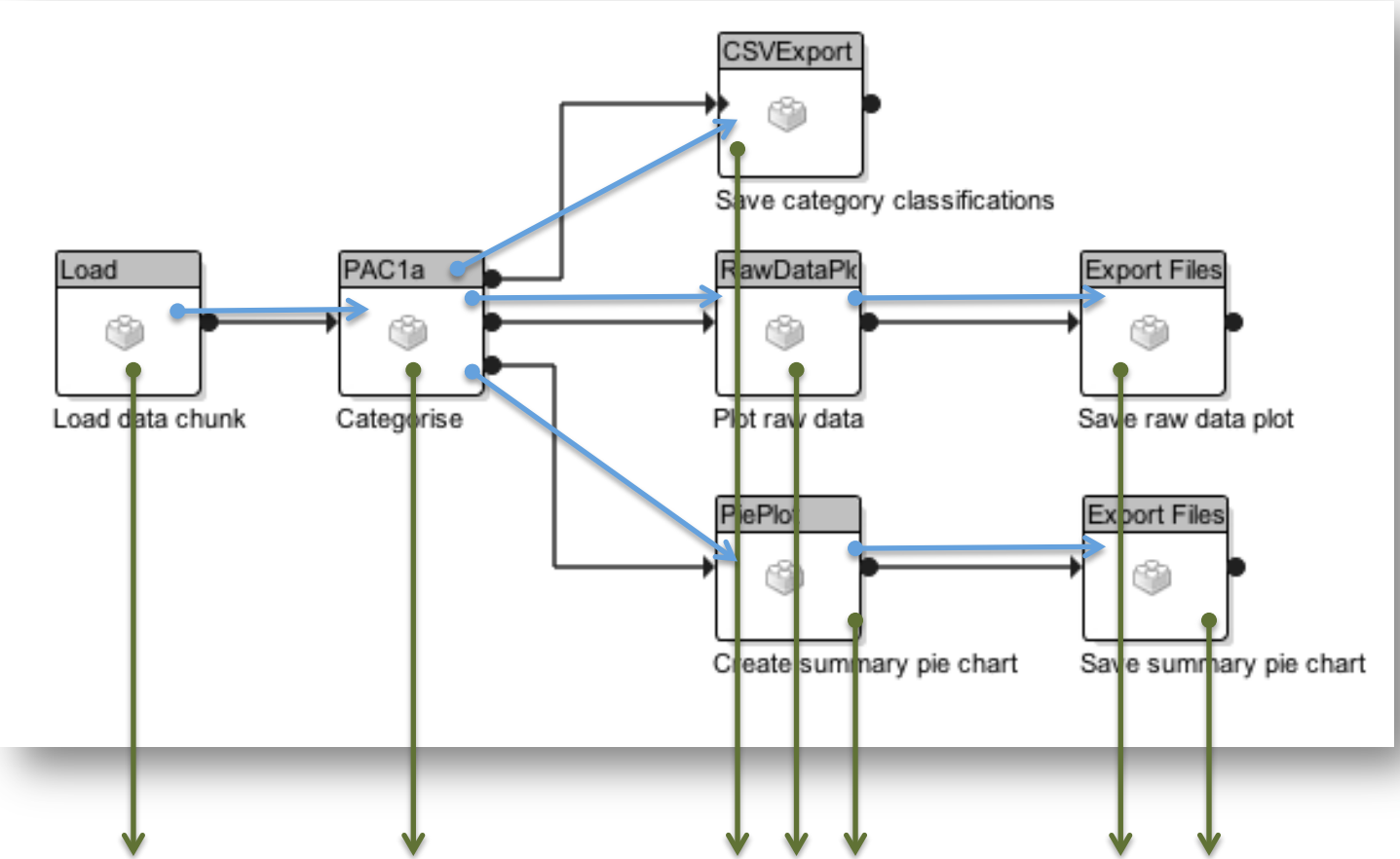
e-science central

Newcastle University

Data volume produced by a block



Propagation of data sizes



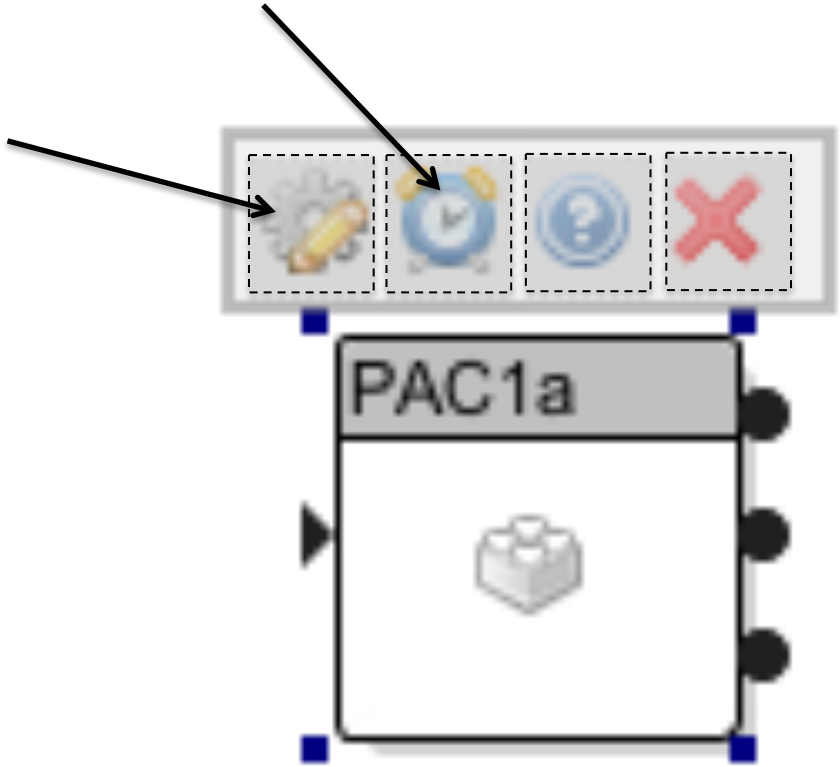
e-science central

Newcastle University

Configuring a workflow Block

Select the version of the block

Configure block

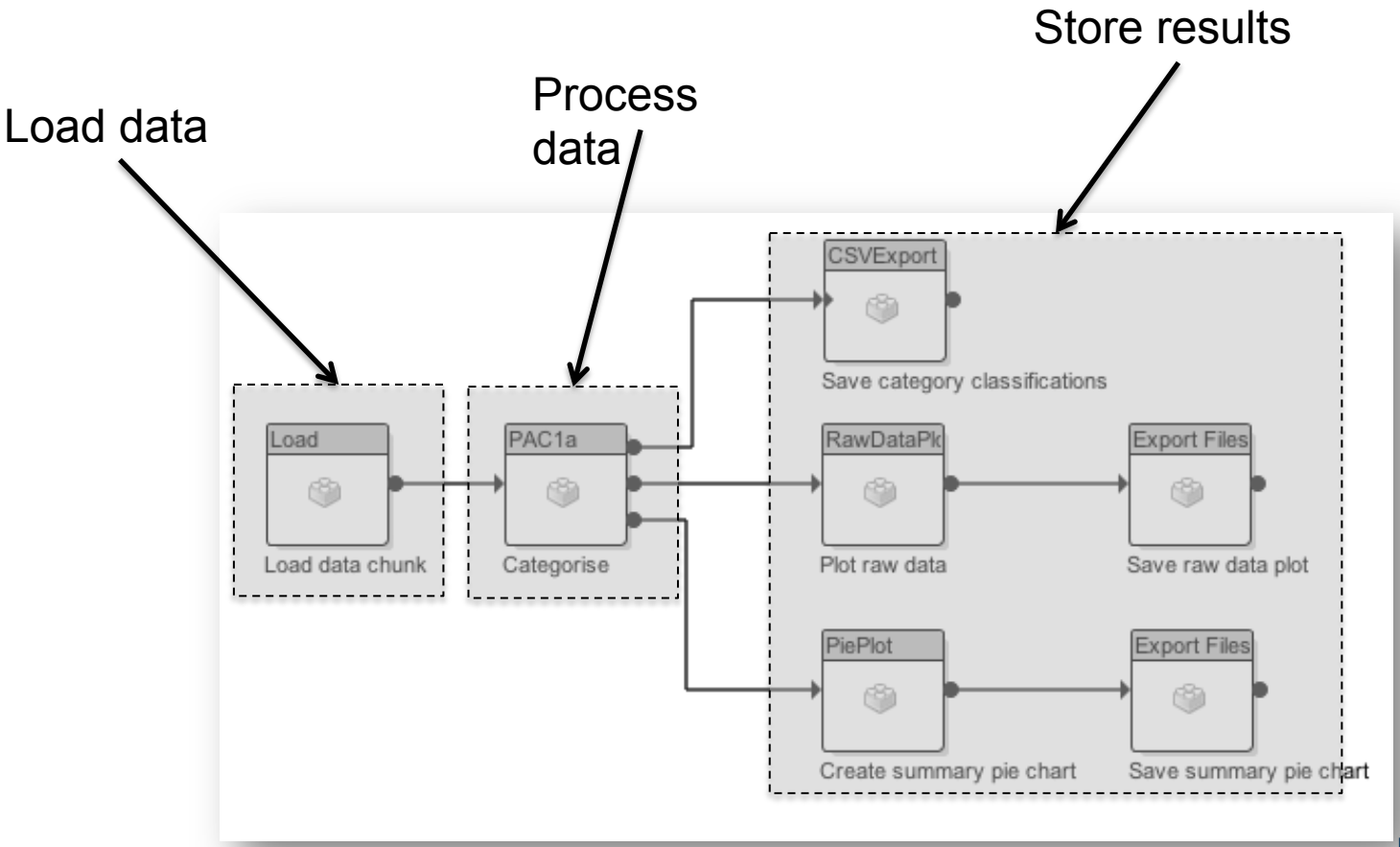


e-science central

Newcastle University

Anatomy of a workflow

Typical simple workflow – follows the standard pattern



e-science central

Newcastle University

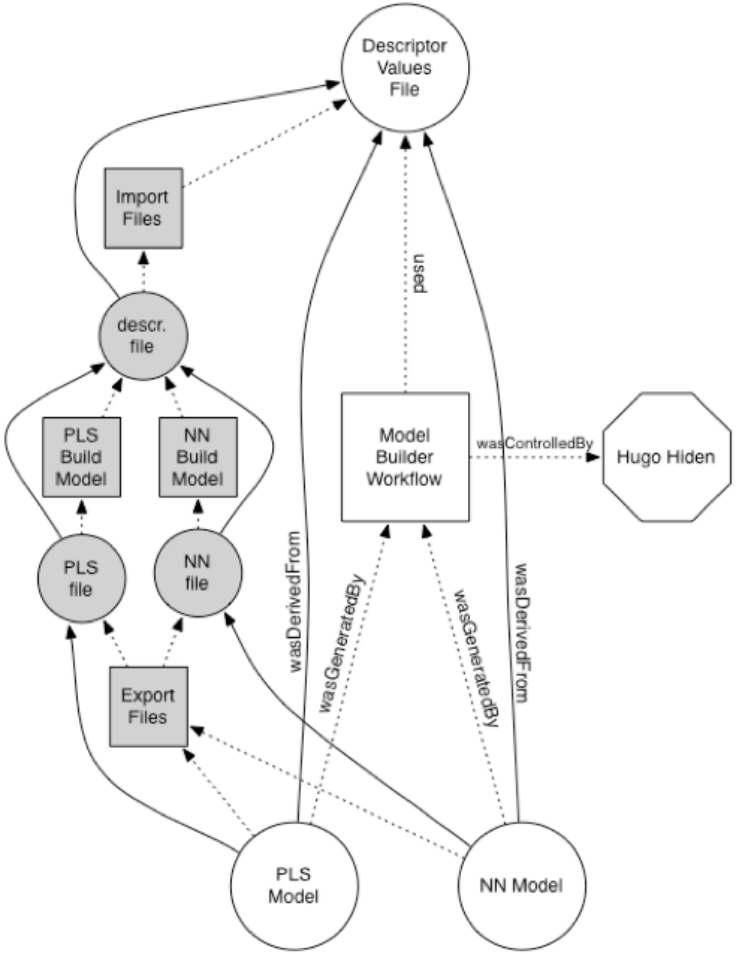
Provenance/Audit Requirements

- How was data generated?
  - What algorithm?
  - What version?
- Are these results reproducible?

- How have bugs manifested?
  - Which data affected
  - How do we regenerate affected data?
- Performance Characteristics
- How do we deal with new data?

Provenance Model

- Based on OPM
  - Processes, Artifacts, Agents
- Directed Graph
- Multiple views of provenance
  - Dependent on security privileges

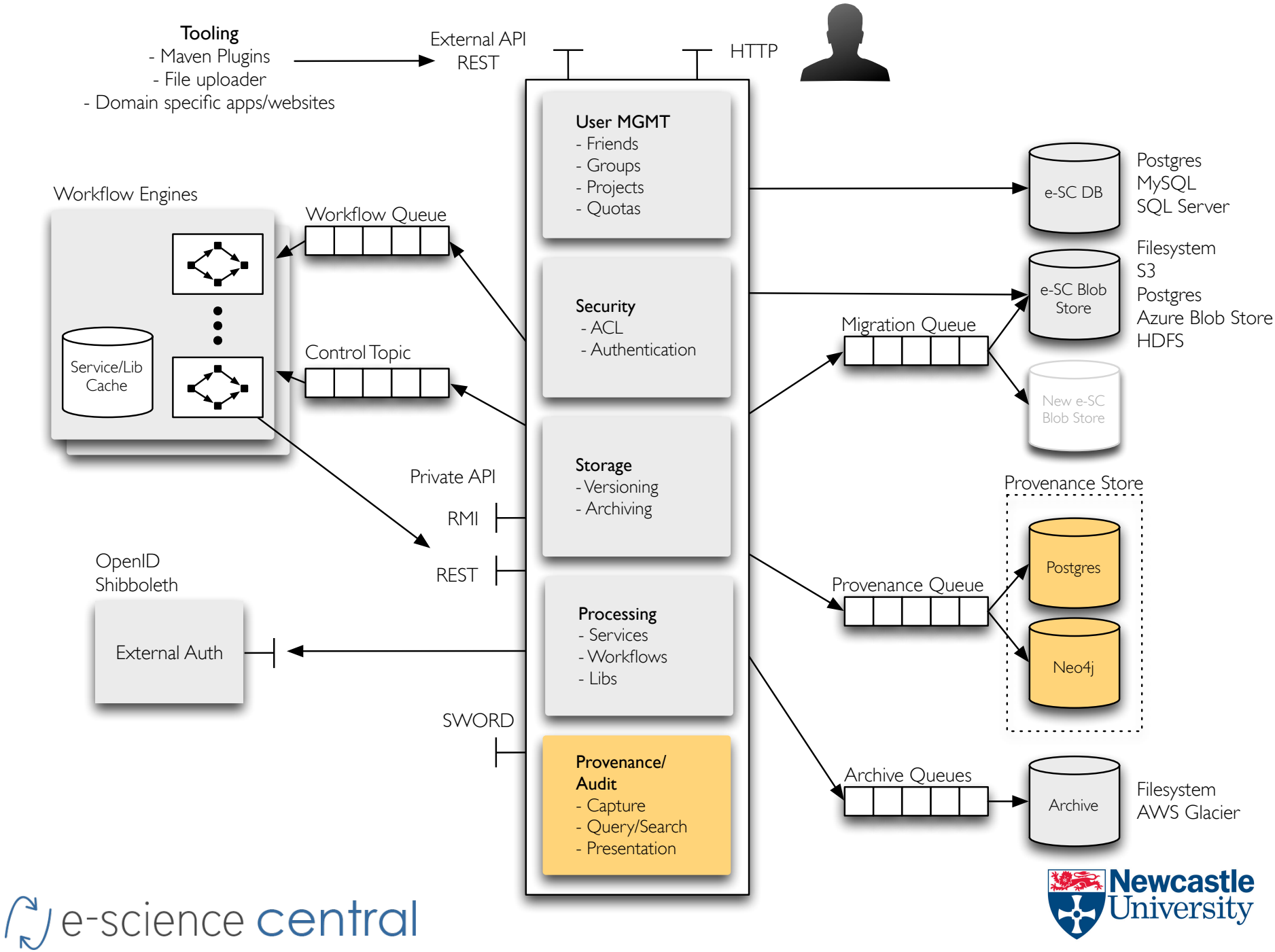


e-science central

Newcastle University

Storing Provenance

- Neo4j
  - Open Source Graph Database
  - Nodes/Relationships + properties
  - Querying/traversing
- Access
  - Java lib for OPM
  - e-SC library built on top of OPM lib
  - REST interface
- Options for HA and Sharding for performance


Tooling
- Maven Plugins
- File uploader
- Domain specific apps/websites
External API
REST
HTTP
User MGMT
- Friends
- Groups
- Projects
- Quotas
Security
- ACL
- Authentication
Storage
- Versioning
- Archiving
Processing
- Services
- Workflows
- Libs
Provenance/
Audit
- Capture
- Query/Search
- Presentation
Workflow Engines
Service/Lib
Cache
Workflow Queue
Control Topic
Private API
RMI
REST
OpenID
Shibboleth
External Auth
SWORD
e-SC DB
Postgres
MySQL
SQL Server
e-SC Blob
Store
Filesystem
S3
Postgres
Azure Blob Store
HDFS
Migration Queue
New e-SC
Blob Store
Provenance Store
Postgres
Neo4j
Provenance Queue
Archive Queues
Archive
Filesystem
AWS Glacier
e-science central
Newcastle
University

Workflow Blocks

- Workflow blocks are units of code that execute as part of a workflow
  - They have a defined structure
  - Can be configured using properties
    - Strings, numbers, booleans, file references, lists etc
  - Can act on local files, data-sets, name-value pairs, serialized Java objects and links to files stored in e-SC
  - Need to be able to operate without user interaction

Execution of Workflow Blocks

- Blocks execute as part of a workflow
  - The code is transferred to the machine executing the workflow
  - The block code is unpacked on the workflow machine
  - Dependencies are also downloaded and unpacked
  - The block is then executed in the workflow working directory
    - Properties are assigned
    - Initialisation code is executed
    - The block main code is then executed (potentially multiple times)
    - Termination code is then executed

Accessing the e-SC Server

- Java and JavaScript blocks have access to an API that provides limited access to information held in the e-SC server
  - Upload / download files
  - Attach / read metadata
  - Update / query datasets
  - Execute additional workflows
- Actions performed using the API are carried out as the same user executing the workflow

Case Studies

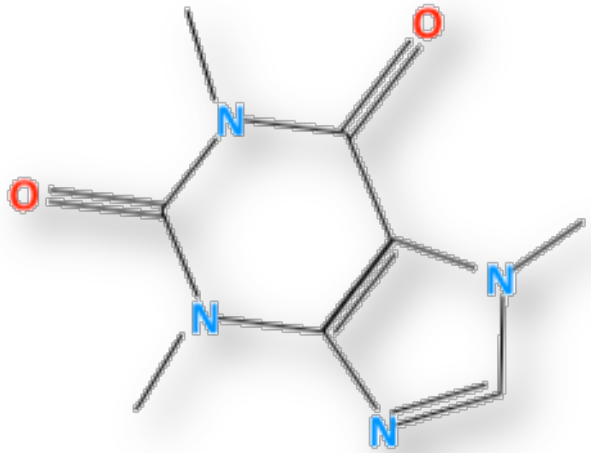
e-science central

Newcastle University

QSAR - The Problem

What are the properties of this molecule?

Toxicity



Biological Activity

Solubility

Perform experiments

Time consuming

Expensive

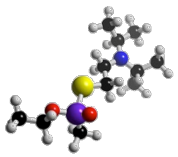
Ethical constraints

e-science central

Newcastle University

QSAR

Quantitative Structure Activity Relationship

Activity ≈ *f(*  *)*

More accurately, Activity related to a *quantifiable* structural attribute

Activity ≈ *f(logP, number of atoms, shape....)*

Currently > 3,000 recognised attributes

http://www.qsarworld.com/

e-science central

Newcastle University

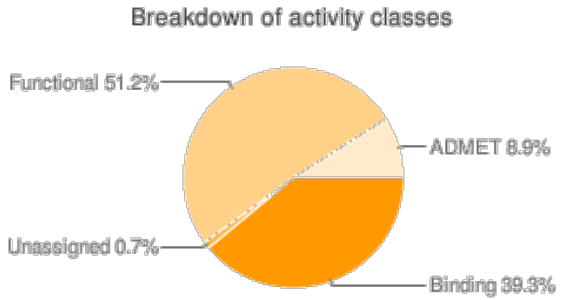
The Alternative to Experiments

Predict likely properties based on similar molecules

CHEMBL Database: data on 622,824 compounds, collected from 33,956 publications

WOMBAT Database: data on 251,560 structures, for over 1,966 targets

WOMBAT-PK Database: data on 1230 compounds, for over 13,000 clinical measurements



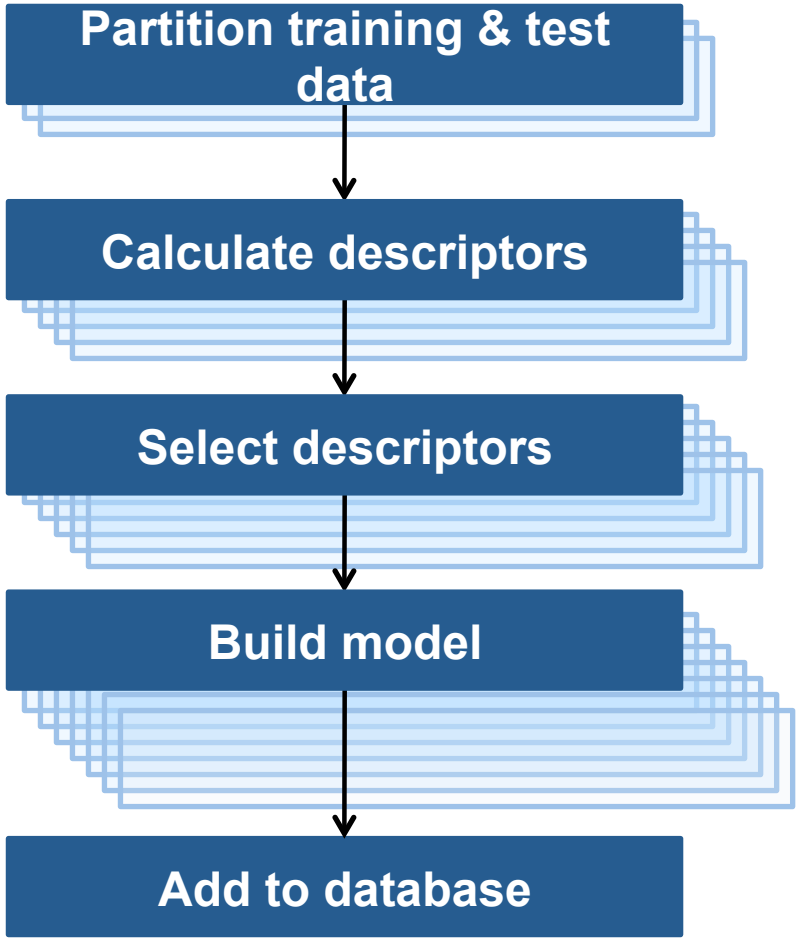
All these databases contain structure information and numerical activity data

What is the relationship between structure and activity?

e-science central

Newcastle University

Branching Workflows



Random split
80:20 split

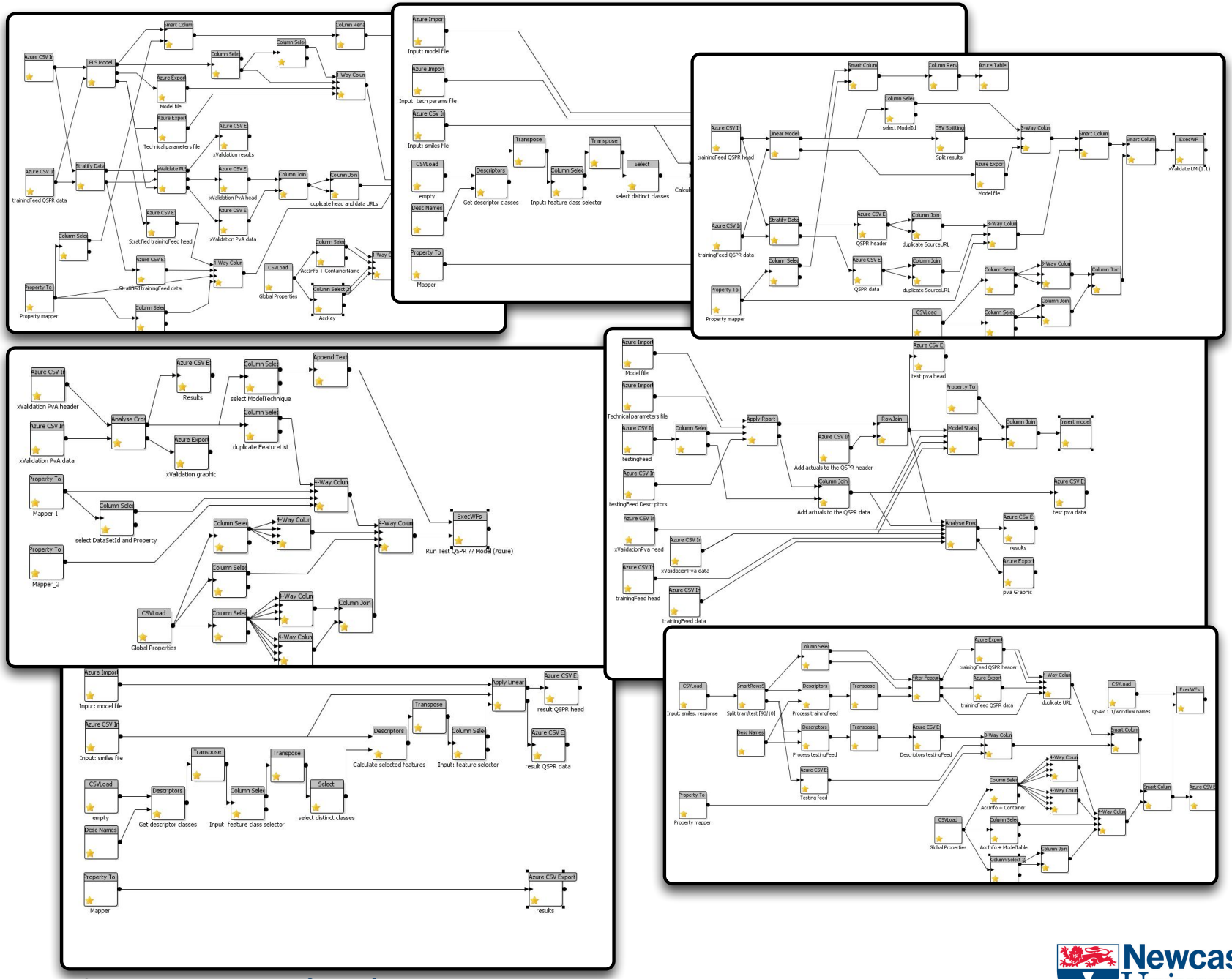
Java CDK descriptors
C++ CDL descriptors

Correlation analysis
Genetic algorithms
Random selection

Linear regression
Neural Network
Partial Least Squares
Classification Trees

e-science central

Newcastle University



e-science central

Newcastle University

Results

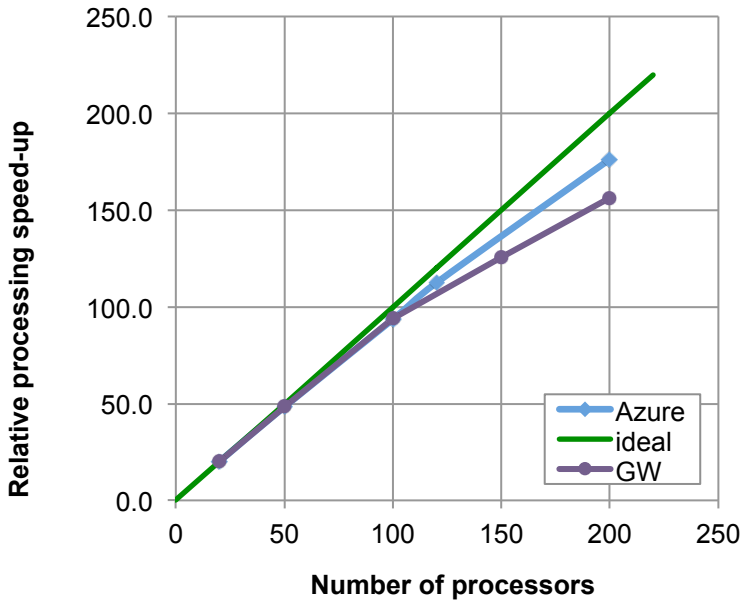
- 250k models
  - Linear Regression
  - PLS
  - RPartitioning
  - Neural Net
- 460K workflow executions
- 4.4M service calls

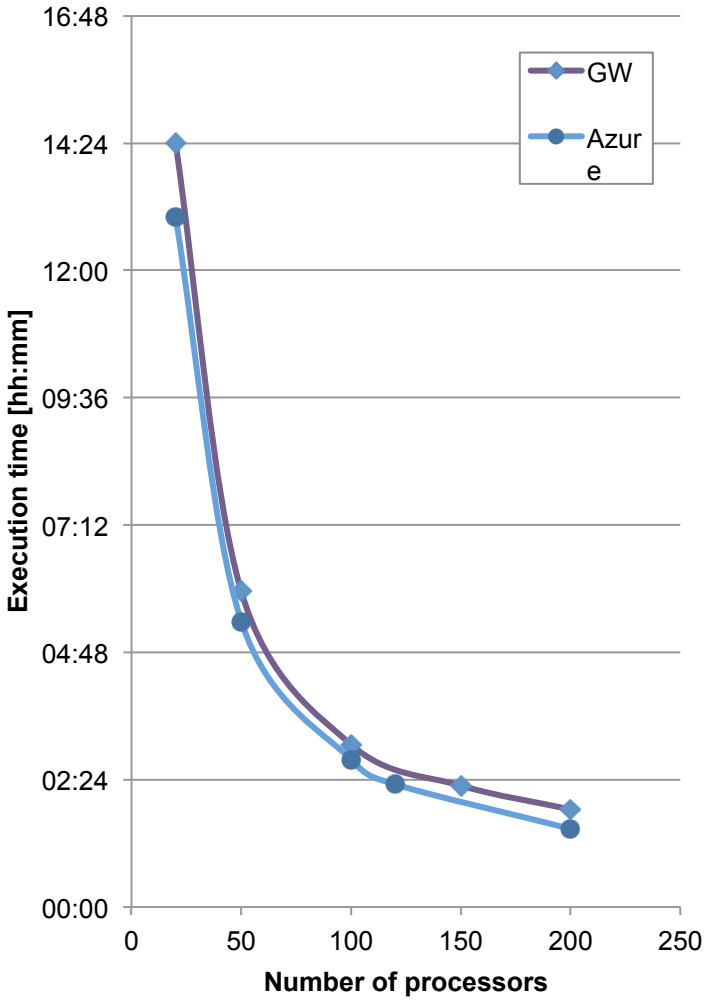
- QSAR Explorer
  - Browse
  - Search
  - Get Predictions

Scalability: Large Scale QSAR

480 datasets sequential time: 11 days

	100 Nodes	200 Nodes
Response Time	3hr 19mins	1hr 50mins
Speedup	94x	156x
Efficiency	94%	78%
Cost	$55.68	$51.84





e-science central

Newcastle University

Performance is great but …

Drug Development requires us to capture the data and the process

MOVEeCloud Project

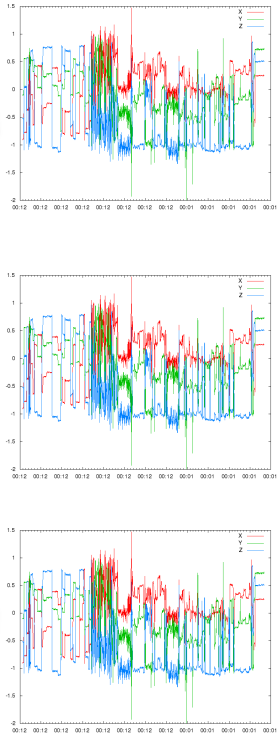
- Investigating the links between physical activity and common diseases – type 2 diabetes, cardiovascular diseas

- Wrist accelerometers worn over period
- Measures movement at 100Hz
- Processing ideal for Azure
  - Bursty data processing as new da
  - Embarrassingly parallel
  - Large datasets

e-science central

Newcastle University

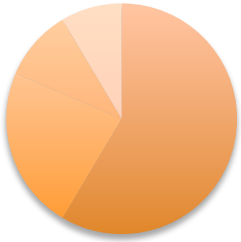
MOVEeCloud Process

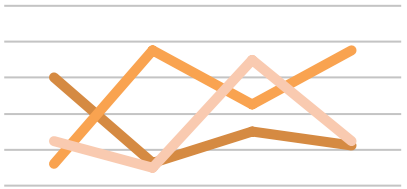


Analysis and Classification

R, Java, Octave

Sleep	Walking	Sedentary	Activity	Sedentary





Clinician's Report

Patient Interventions

Methodology Section for Papers

e-science central

Newcastle University

Data Sizes

100 samples / second	100 rows
3600 seconds / hour	360,000 rows
24 hours / day	8,640,000 rows
7 days / study	60,480,000 rows

/ patient / visit

Cohort size of 800 patients and multiple visits

e-science central

Newcastle University

Working with larger data sets

- As we add more workflow engines server load increases
  - One server can cope 200 engines if files are small
- This is not the case with movement data
  - Only support 4 engines
- Increase the bandwidth to the engines
  - Clustering appserver /database?

HDFS

- Implemented prior to Native HDFS on Azure
- Easy to integrate with e-sc
  - Java system just requires libraries included in e-sc
- Distributed store where bandwidth increases with number of machines
  - Bits of data spread around lots of machines
- Concept of data location
  - Potential to route workflows to execute as close as possible to storage
- Other applications also also built on top of HDFS
  - Open TSDB to store timeseries for movement data

Initial Results

For a single data set processing went from 60 to 16 minutes using 4 workflow engines running HDFS

- 4 engines the limit for one e-sc server
  - Main server hit 100% CPU delivering data
  - No further improvements with more engines
- Using HDFS CPU was consistently below 5%
  - More like our earlier scalability results

- Once data had been chunked processing was the same for each chunk

- The improvement lay entirely in staging and uploading results

Upcoming Challenges

- Process Newcastle 85+ and Whitehall Study Data
  - 6TB
- New TSB Project with RedHat and Arjuna
  - e-Science Central onto OpenShift
  - Integrate Arjuna Agility
  - Analyse traffic flow data from Newcastle

Demo

e-science central

Newcastle University