Running Large Workflows in the Cloud

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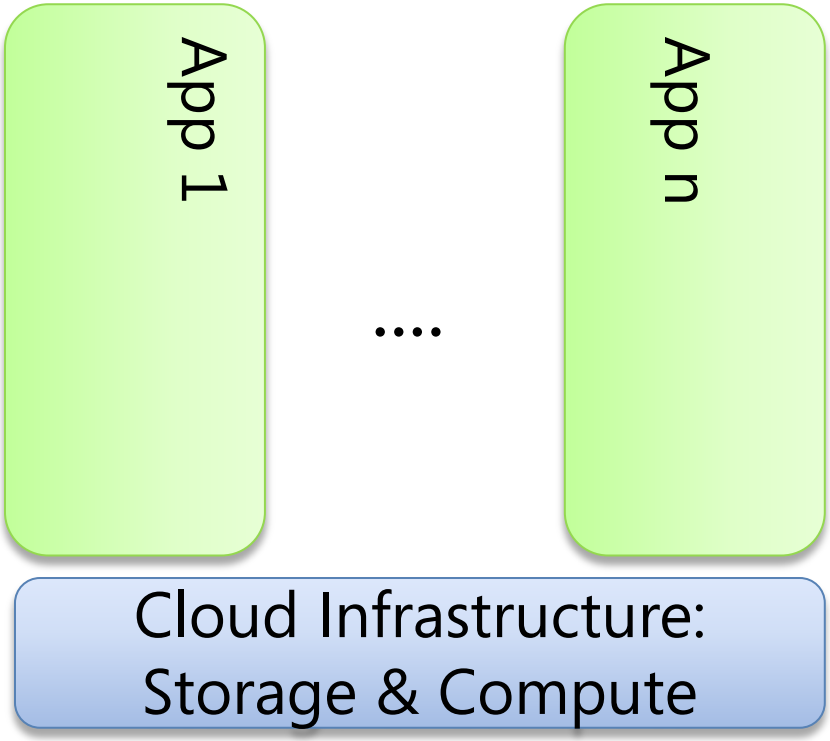
Venus-C
Virtual multidisciplinary EnviroNments USing Cloud infrastructures

The Promise of Clouds

- Reduced capital expenditure
- Reduced Energy
- Scalability
- “On-demand resources”

The Problem with Clouds

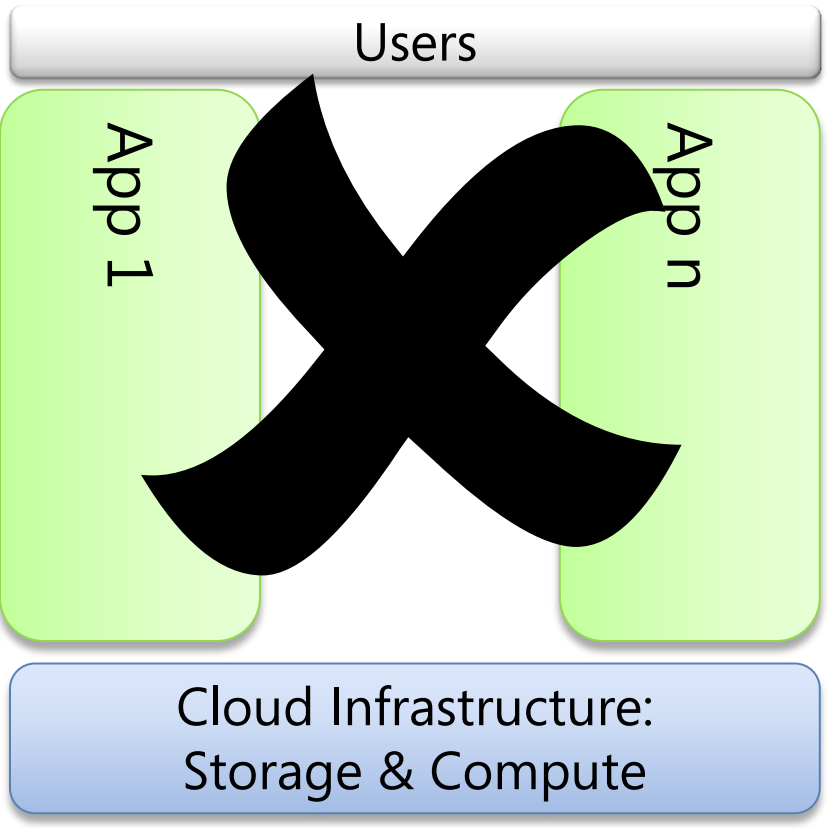


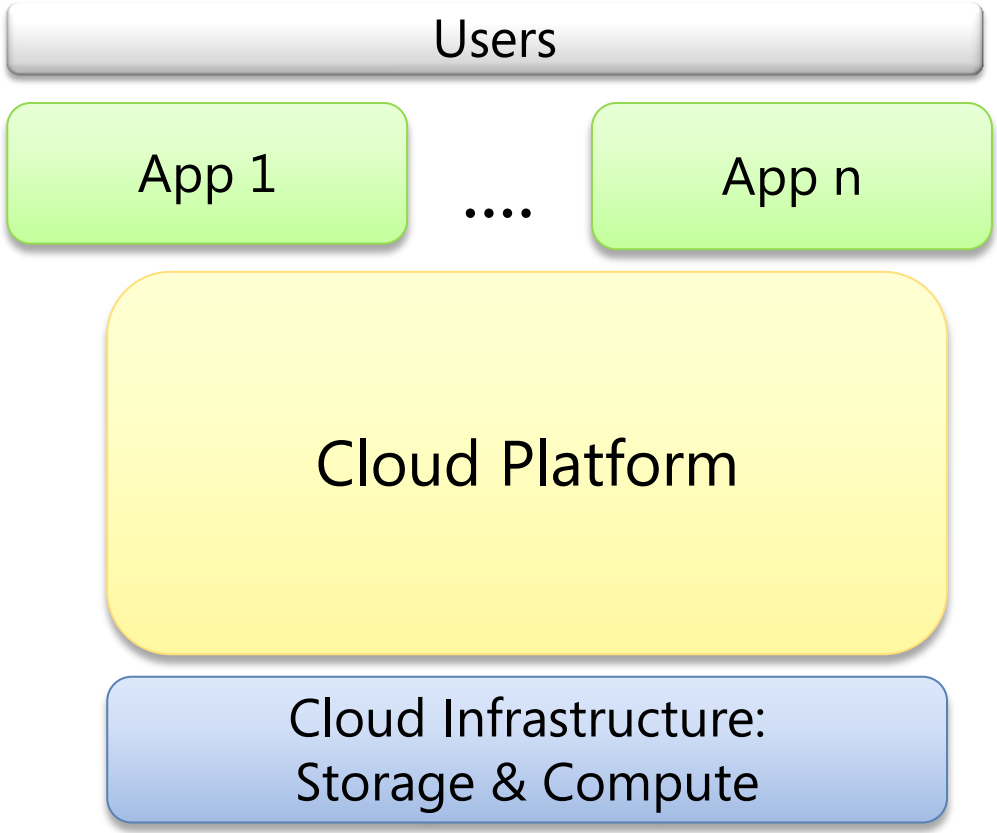
Building scalable, reliable, secure systems on cloud infrastructure is still hard

- *deep IT skills*
- *bespoke*
- *on-going management costs*
- *lock-in*

Realising cloud advantages is beyond most who could benefit

Cloud Options



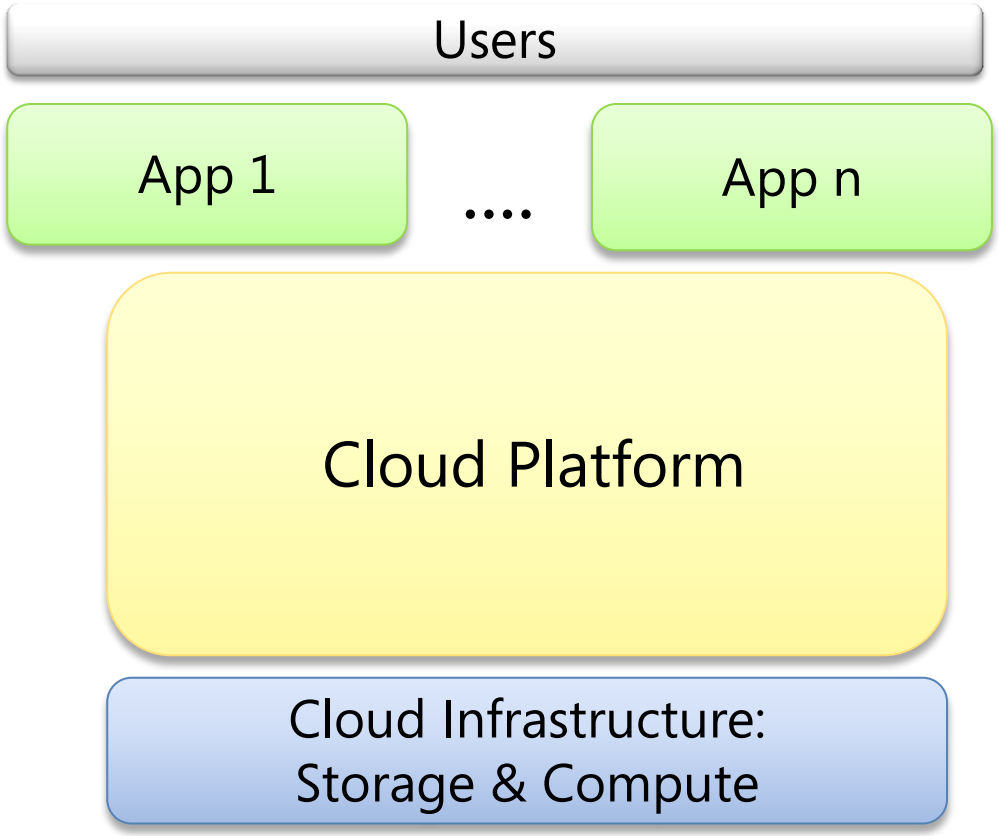


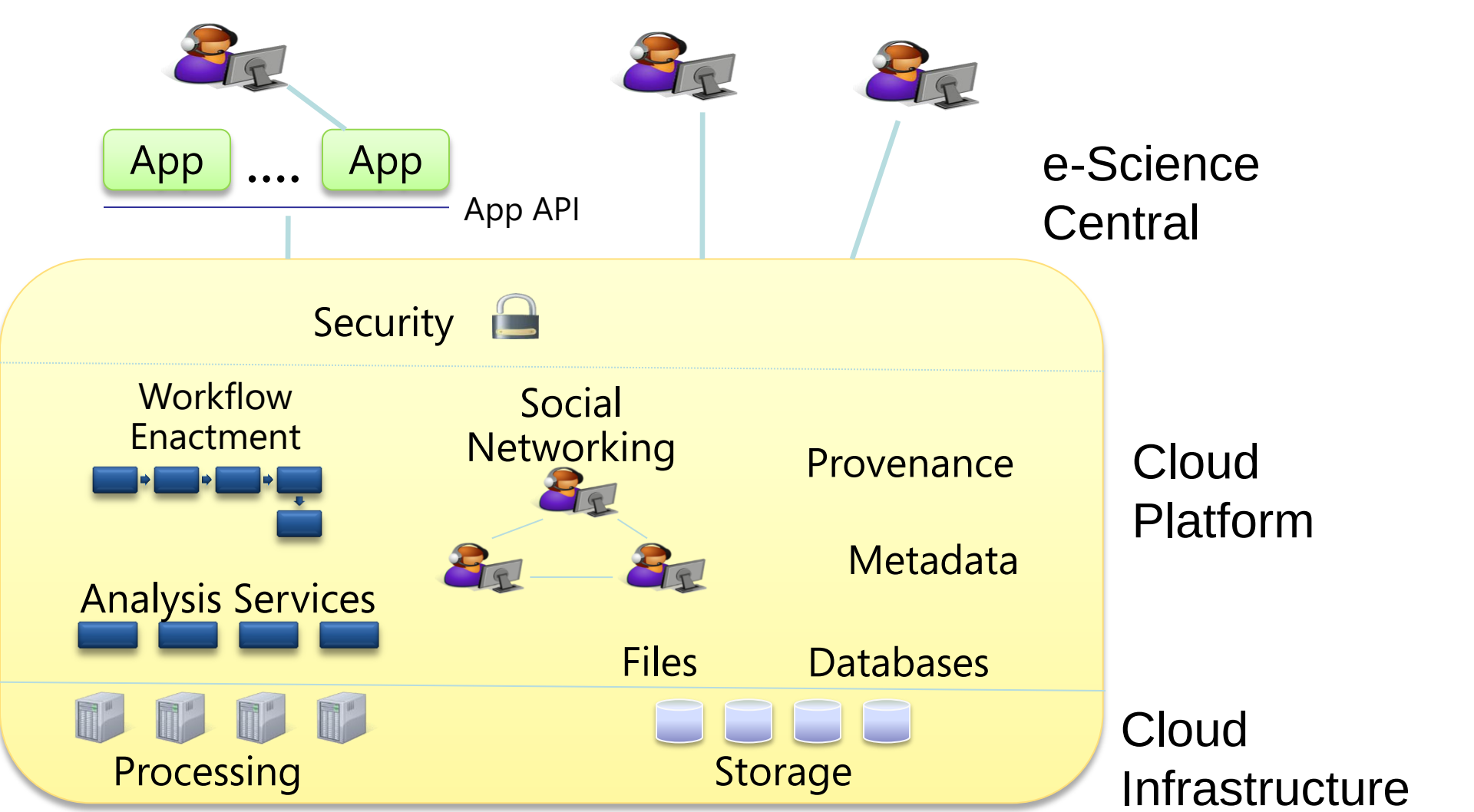
e-Science Central

Science as a Service
for users & programs

Cloud Platform
for developers

Portable: run on
- Azure
- Amazon
- Private Cloud

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Hanani Abang-Ibrahim updated My PhD Research Diary

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John Colquhoun published I am blogging today though :-)

John Colquhoun published I didn't blog yesterday...

d published Week beginning 11th October 2010

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published More teaching and demonstrating

DLL

Hugo Hiden has made commons-math-2.1 public

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Gavin Wood published 25th to 29th October 2010

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Version 1 : 08 Mar 2010 10:17

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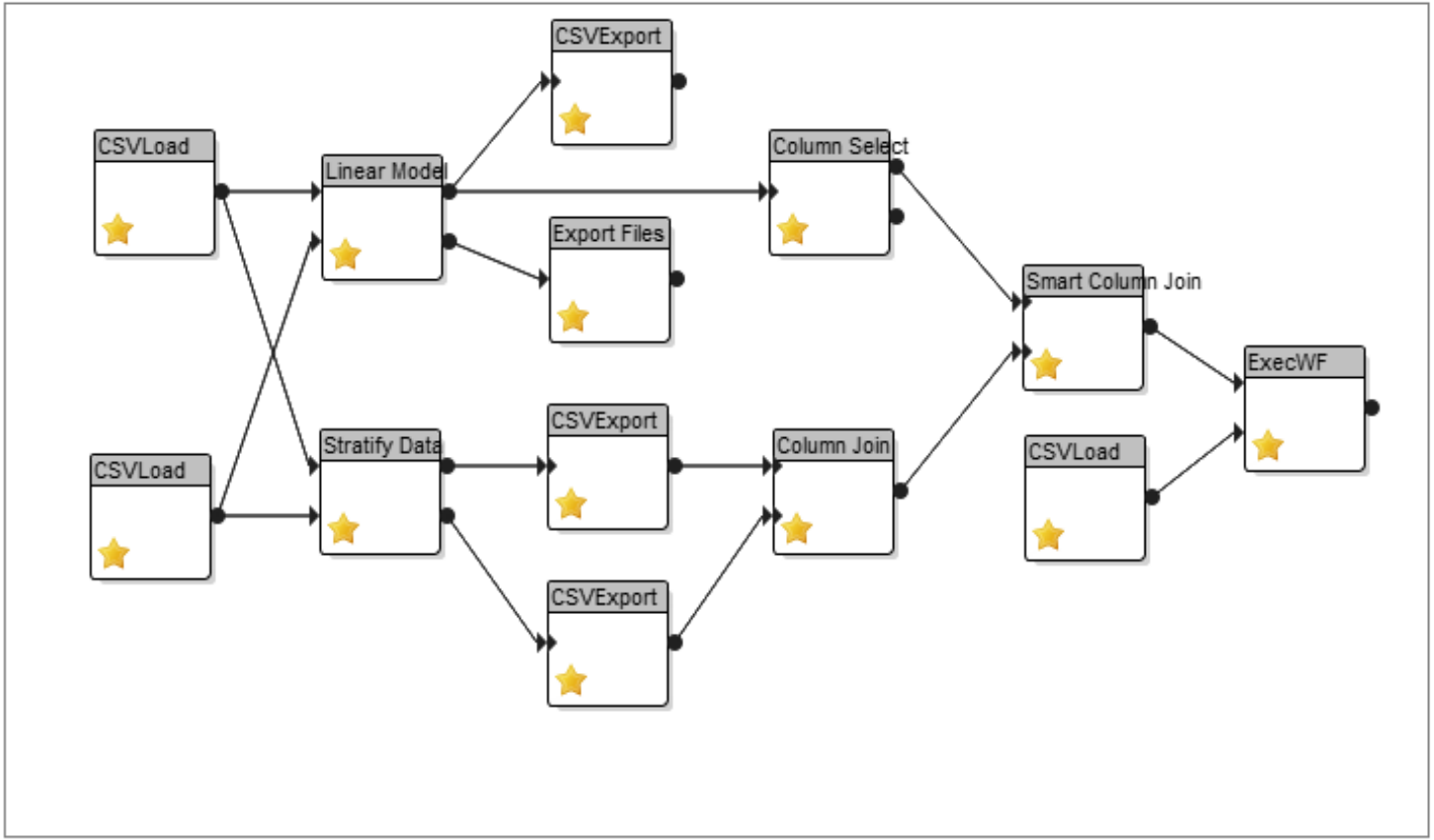
Joanna Berry	read,write
Stephen McGough	read

Workflow Editor

1: May 26, 2011 4:04:55 PM | Help | Properties | Run | Delete Selected | Save

- **Discovery Bus**
  - RPart Model
  - Neural Net Model
  - xValidateNNM
  - xValidatePLSM
  - Linear Model
  - xValidateRPartM
  - xValidateLM
  - StratifyData
  - PLS Model
  - Filter Features
- **File Management**
- **Import**
- **Workflow**
- **Windows Azure**
- **Manipulation**
- **Numerical**
- **Chemistry**
- **Export**



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e-Science Central. Science. On Demand.. - Windows Internet Explorer

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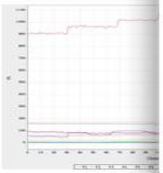
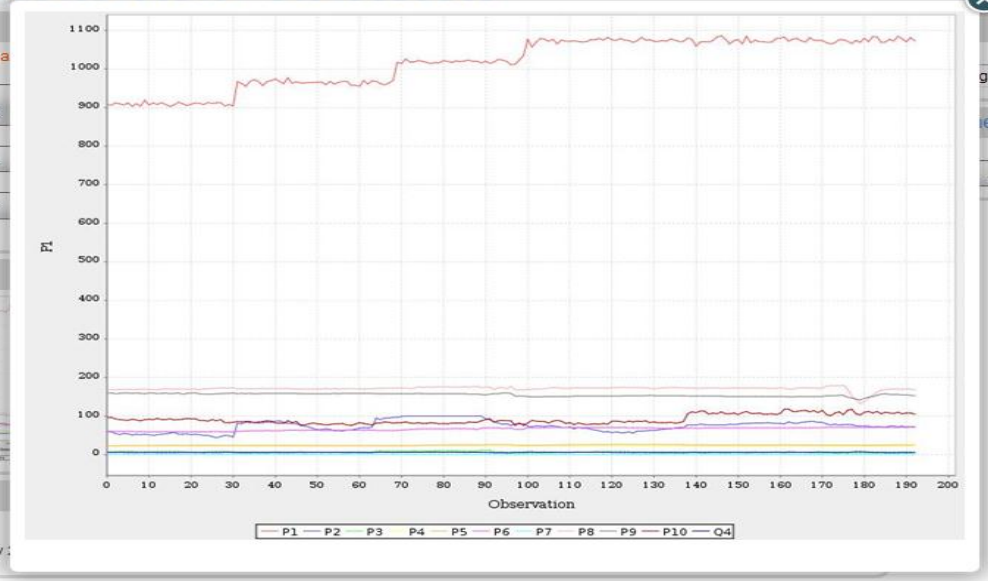


Versions

Version 0: 28 Nov



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28 November 2008: Created by Paul Watson (1)

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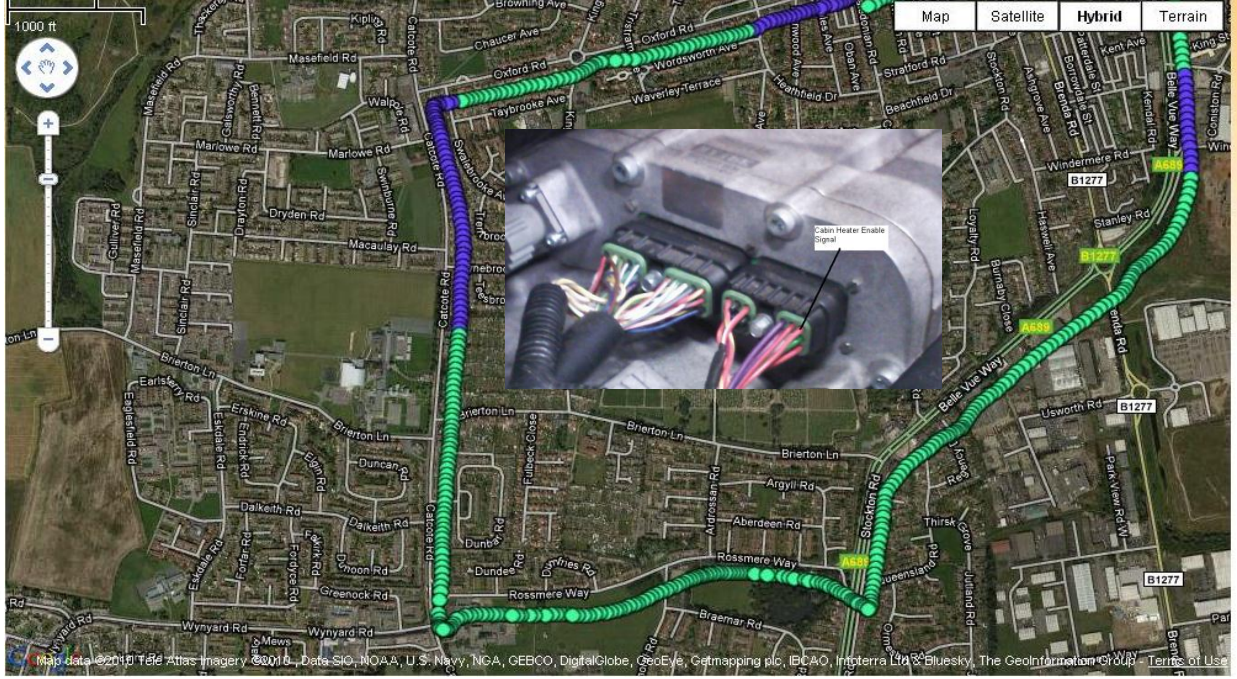
Used for variety of research:

- activity recognition
- spectroscopy
- driving analysis
- chemistry…

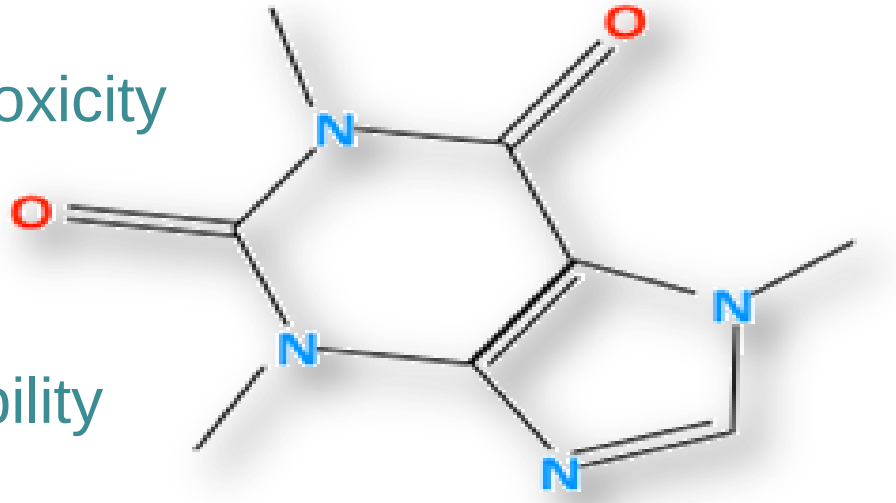


Chemists want to know:

Q1. What are the properties of this molecule?

Toxicity

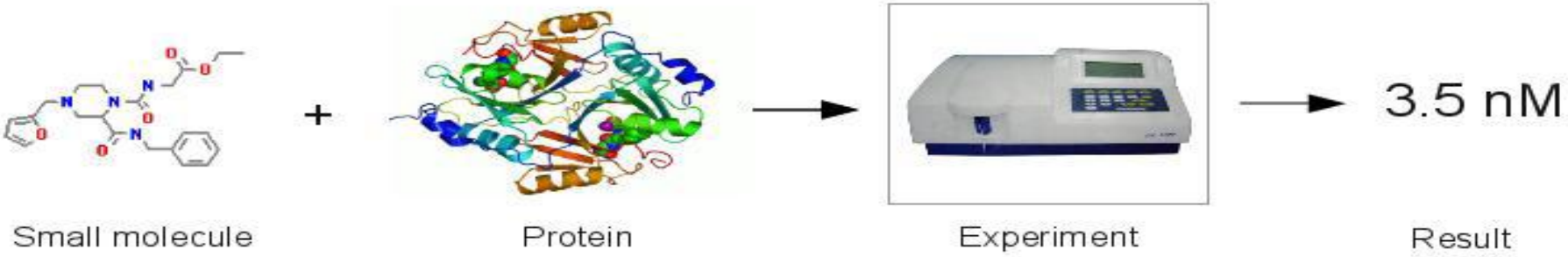
Biological Activity



Solubility

Q2. What molecule would have aqueous solubility of 0.1 µg/mL*?*

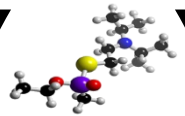
Answering the Question by performing experiments



..... time consuming, expensive, ethical Issues

An alternative to experimentation: QSAR

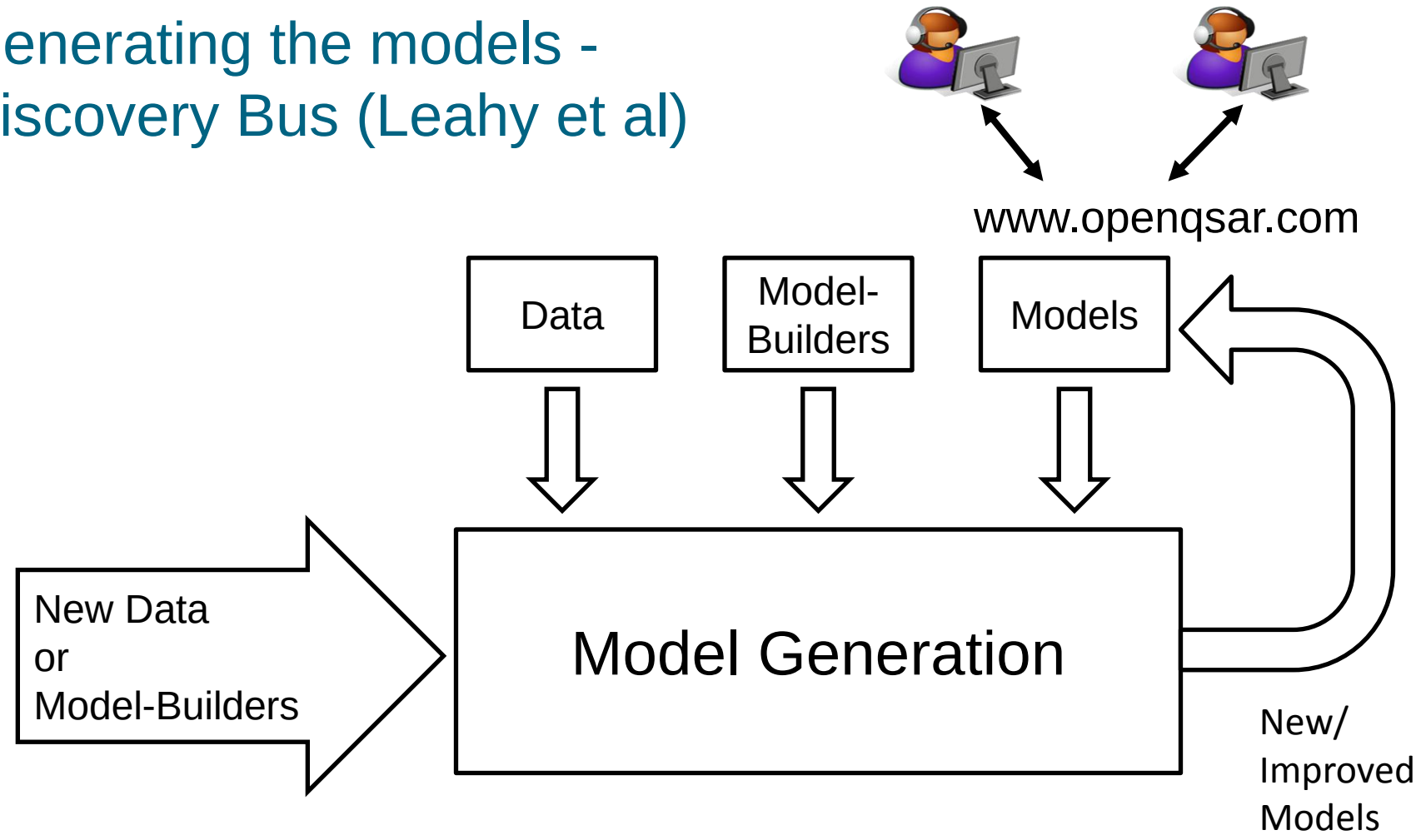
Quantitative Structure Activity Relationship
- predict properties based on similar molecules

$$Activity \approx f(\text{  })$$

quantifiable structural attributes, e.g.

#atoms
logp
shape
.....

Generating the models - Discovery Bus (Leahy et al)



Increasing amounts of data for model building...

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

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

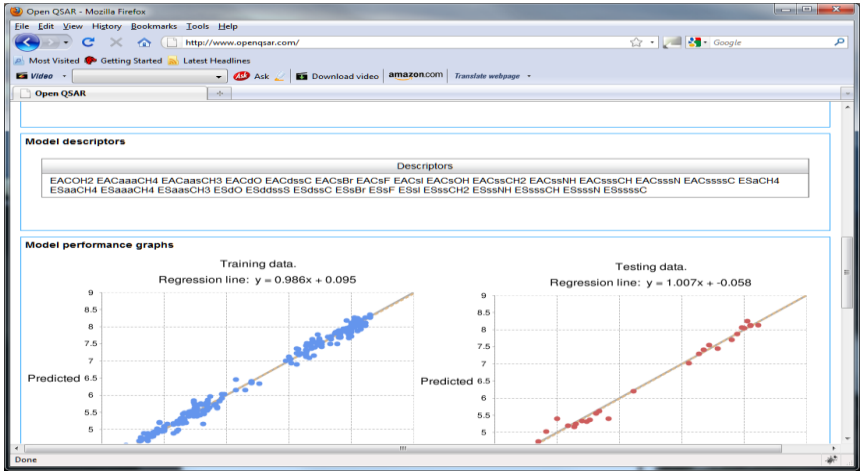
WOMBAT-PK: data on 1230 compounds,
for over 13,000 clinical measurements

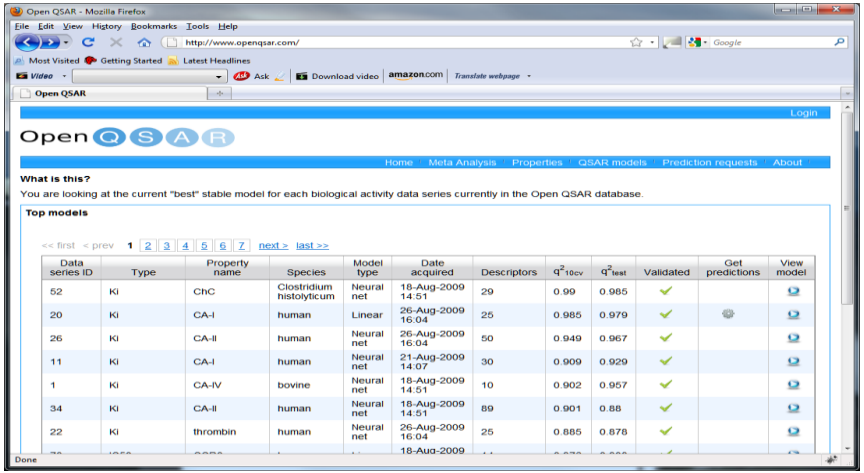
✓ More models
✓ Better models

✗ est. 5 years to process new datasets on existing server

JUNIOR Project Aim

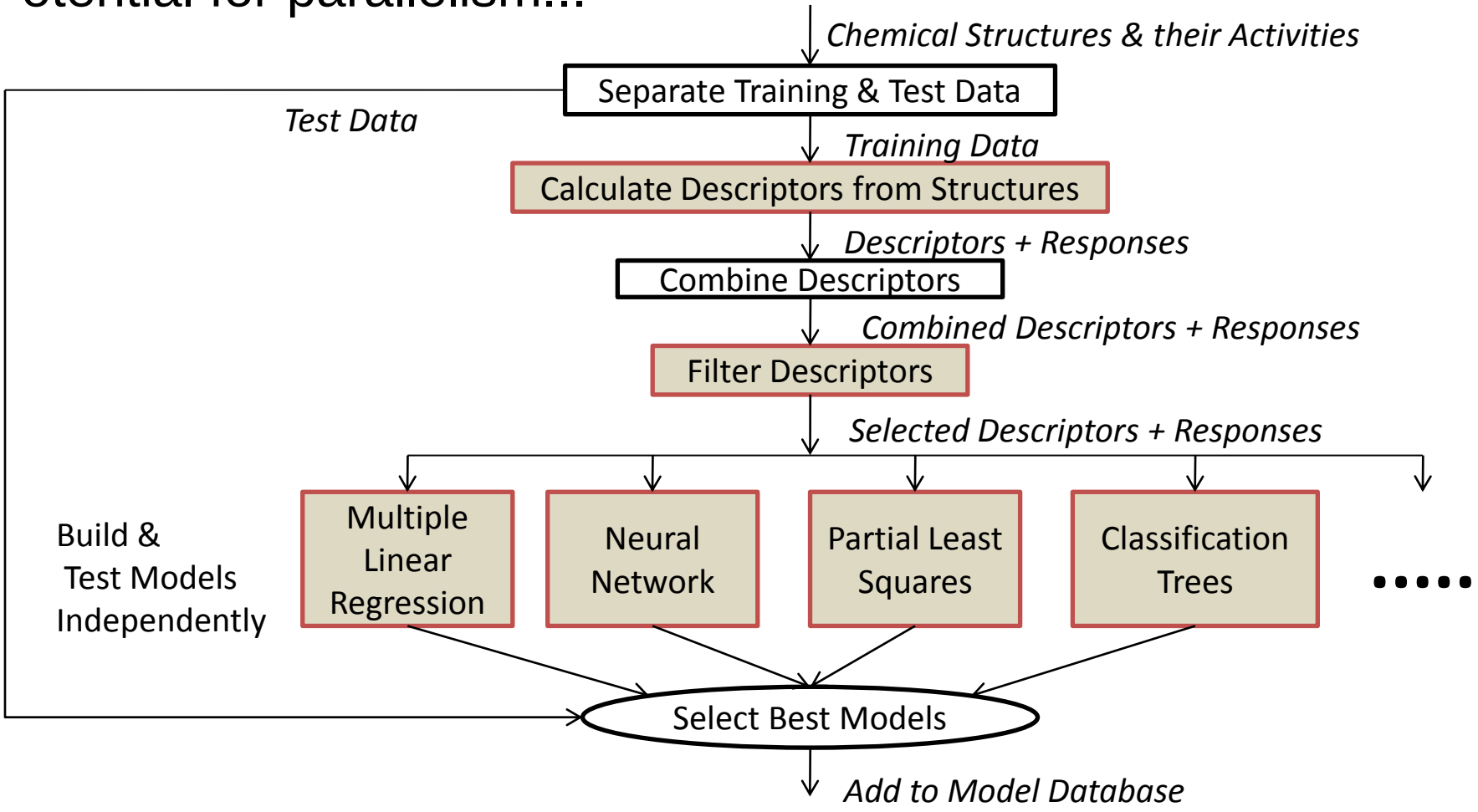
Use Azure to generate models in weeks not years





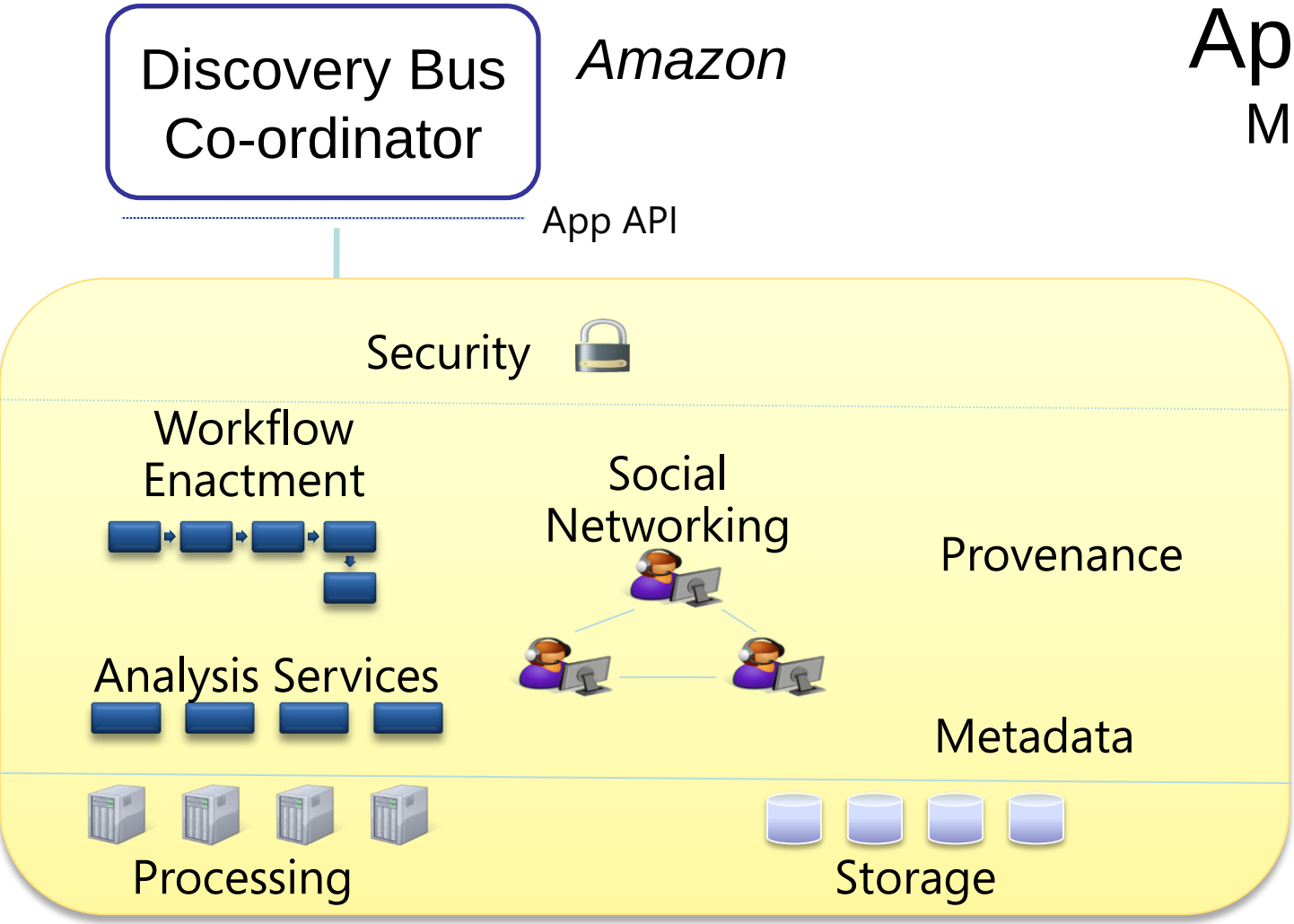
Data series ID	Type	Property name	Species	Model type	Date acquired	Descriptors	q^2_{10cv}	q^2_{test}	Validated	Get predictions	View model
52	Ki	ChC	Clostridium histolyticum	Neural net	18-Aug-2009 14:51	29	0.99	0.985	✓		
20	Ki	CA-I	human	Linear	26-Aug-2009 16:04	25	0.985	0.979	✓		
26	Ki	CA-II	human	Neural net	26-Aug-2009 16:04	50	0.949	0.967	✓		
11	Ki	CA-I	human	Neural net	21-Aug-2009 14:07	30	0.909	0.929	✓		
1	Ki	CA-IV	bovine	Neural net	18-Aug-2009 14:51	10	0.902	0.957	✓		
34	Ki	CA-II	human	Neural net	18-Aug-2009 14:51	89	0.901	0.88	✓		
22	Ki	thrombin	human	Neural net	26-Aug-2009 16:04	25	0.885	0.878	✓		

Potential for parallelism...

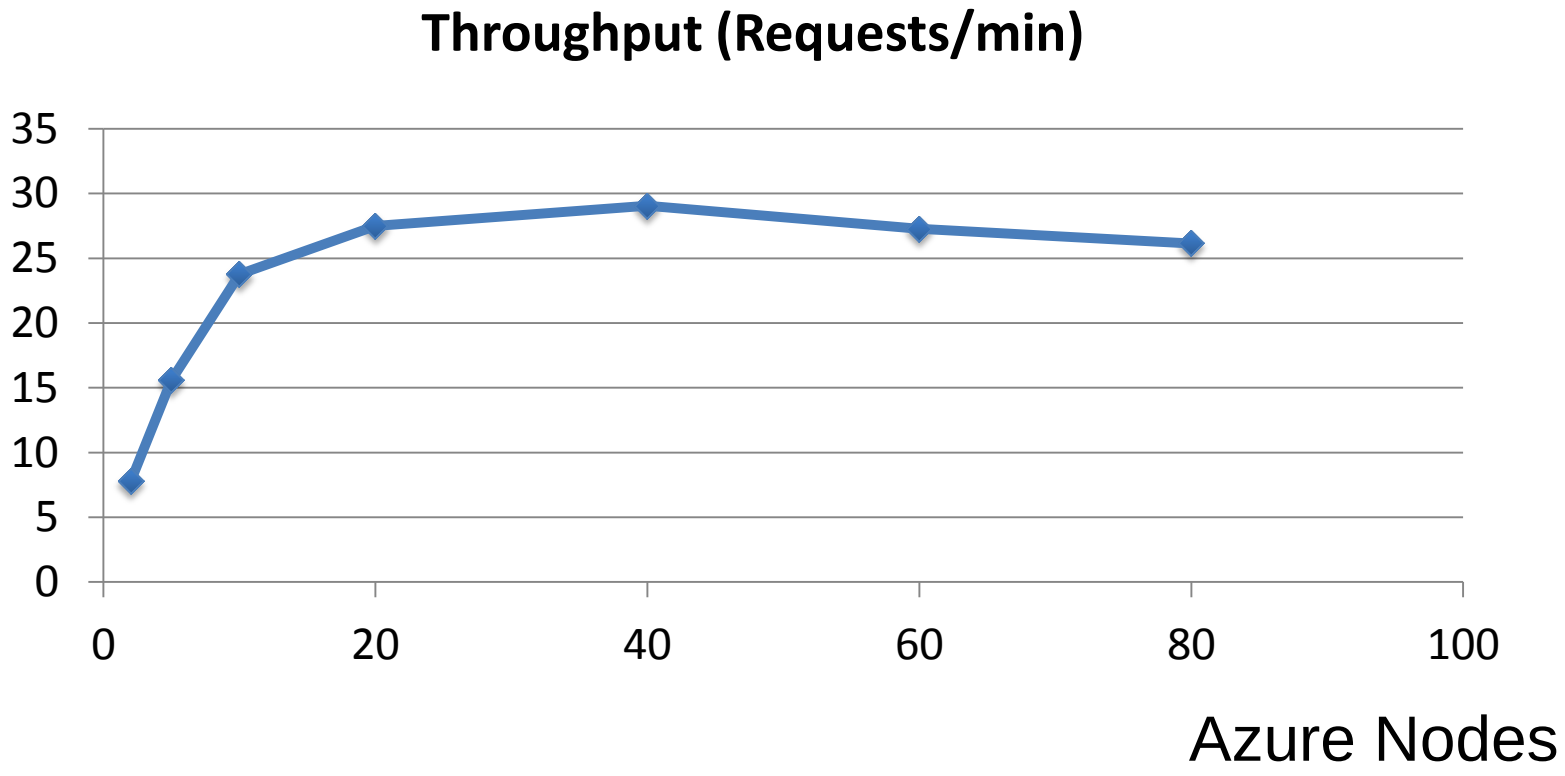


Approach #1

Minimal change to Discovery Bus

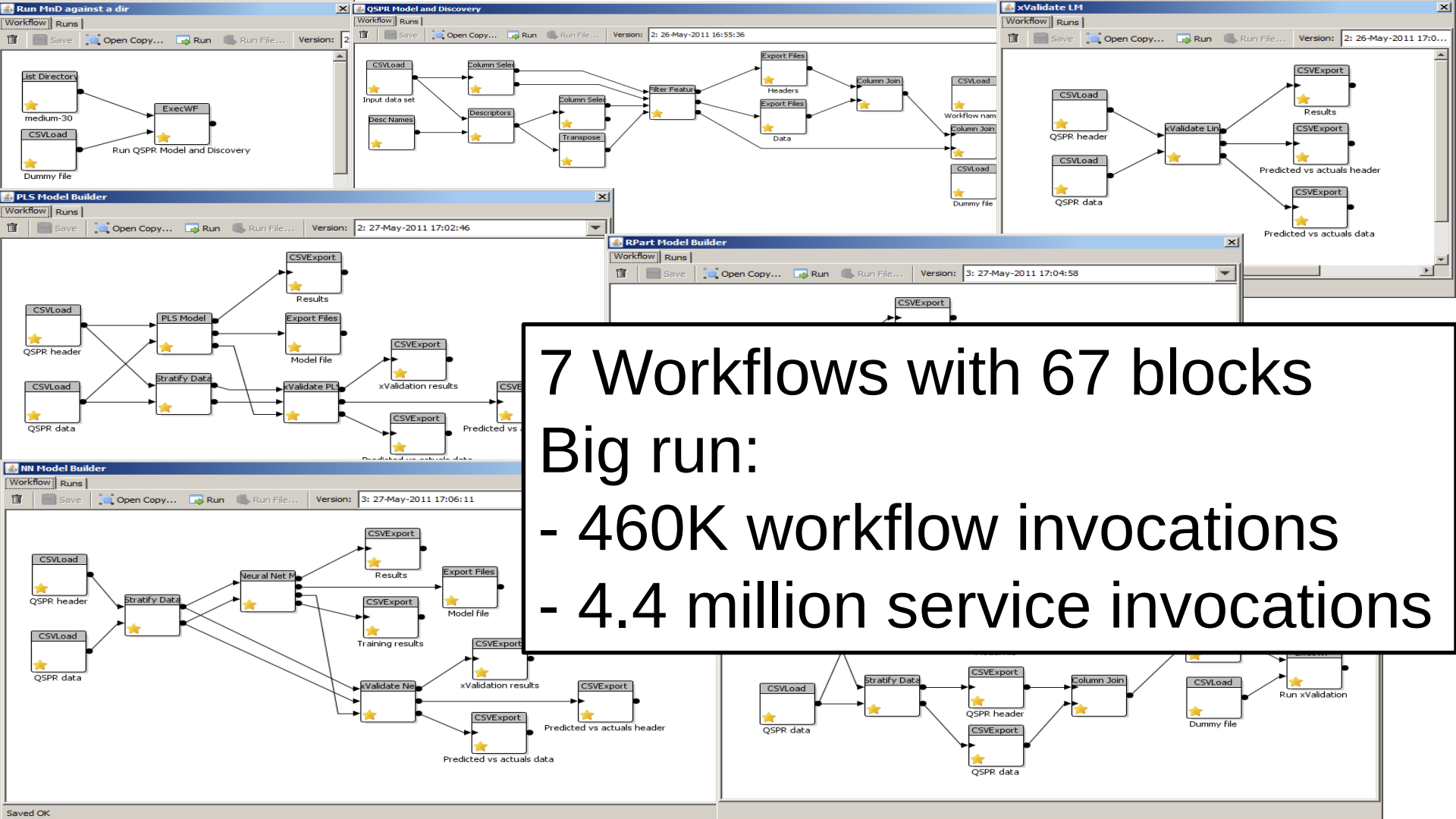


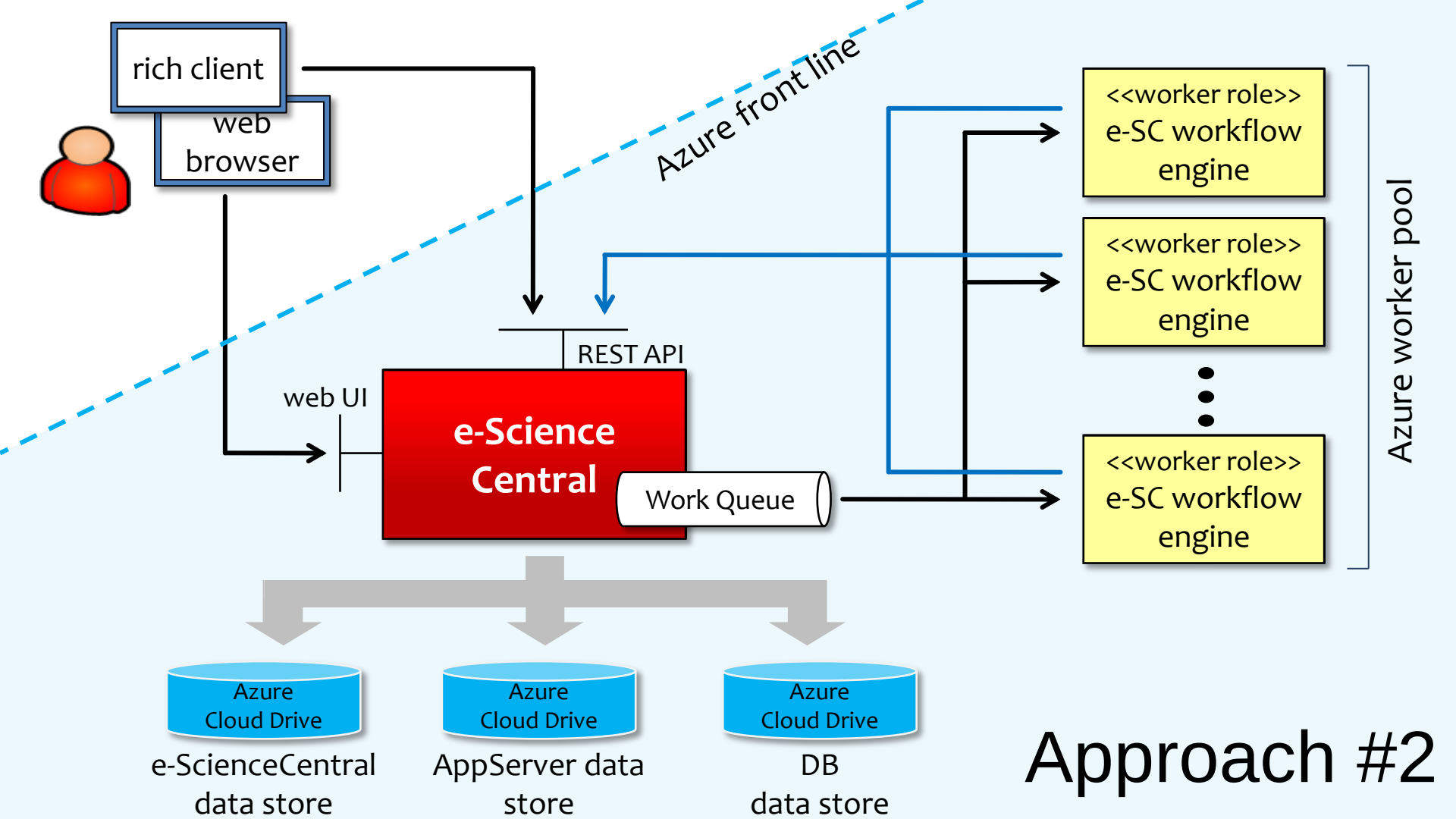
Succeeded in reducing time from (est.) 5 years to 3 weeks, but…



Approach #2

- run entirely within Azure
  - through e-Science Central on Azure


Run MnD against a dir
QSPR Model and Discovery
xValidate LM
PLS Model Builder
RPart Model Builder
NN Model Builder
7 Workflows with 67 blocks
Big run:
- 460K workflow invocations
- 4.4 million service invocations


rich client
web browser
Azure front line
<<worker role>>
e-SC workflow engine
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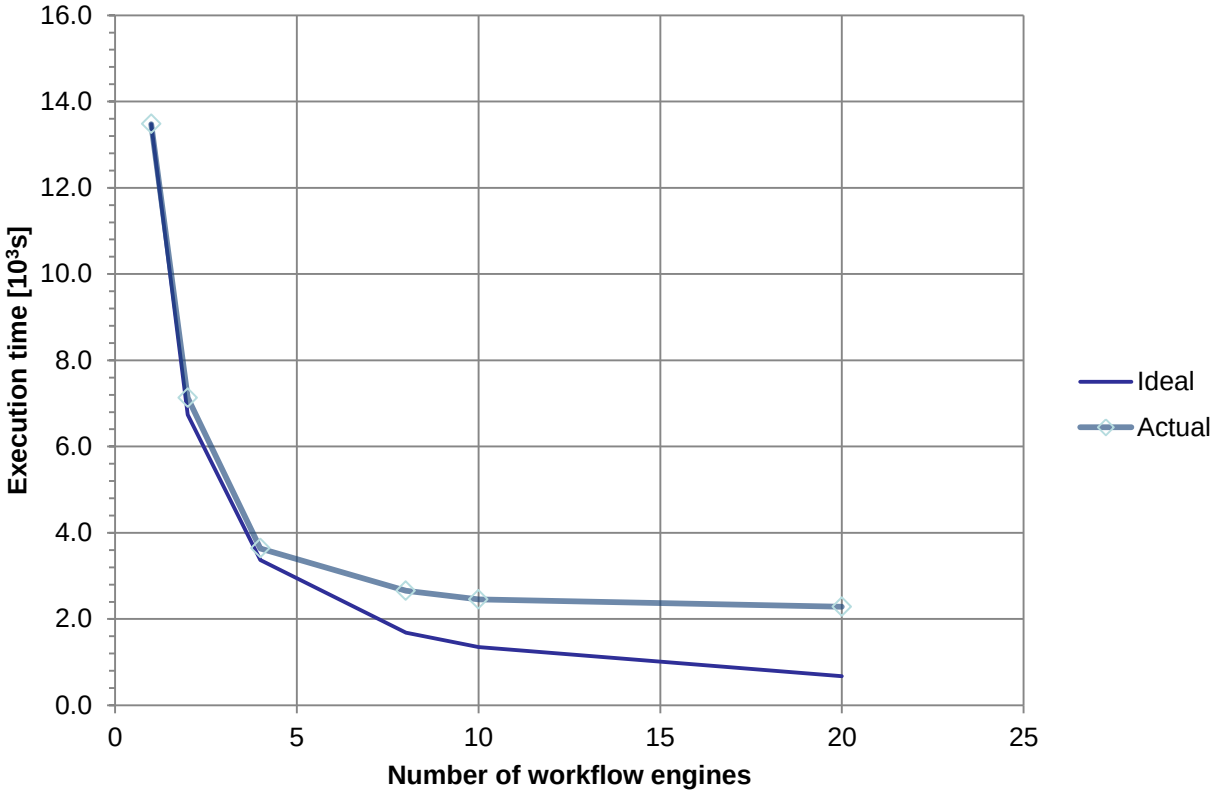
e-SC workflow engine
<<worker role>>
e-SC workflow engine
Azure worker pool
REST API
web UI
e-Science Central
Work Queue
Azure Cloud Drive
Azure Cloud Drive
Azure Cloud Drive
e-ScienceCentral data store
AppServer data store
DB data store
Approach #2

Early Results

- Reduces time to 9 days
  - 5yrs $\rightarrow$ 22 days $\rightarrow$ 9 days
  - but room for improvement….

Scalability



Summary

- *Discovery Bus* exemplifies a good Cloud pattern
  - large, variable, bursty requirements
- e-Science Central is a scalable, secure, portable cloud platform for Azure (and Amazon, and Private Clouds)
- next steps
  - optimize large workflow scheduling
  - automatically adapt #workers