Information Systems, Computing and Mathematics

*Advances in e-Science and e-Research:*

# e-Infrastructures for Modelling and Simulation

Simon J E Taylor

*Editor-in-Chief, Journal of Simulation*

*Chair, SISO CSPI PDG*

*Head, ICT Innovation Group*

Department of Information Systems and Computing

Brunel University

West London, UK

www.brunel.ac.uk/~csstsjt, simon.taylor@brunel.ac.uk

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ICT Innovation Group

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# Cyberinfrastructures for Modelling and Simulation


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ICT Innovation Group

# Presentation Key Question

- Significant investment in e-Infrastructures has brought about a step change in research in areas such as physics, biology and medicine
- What benefits can e-Infrastructure technological advancements bring to Modelling and Simulation?

# Overview

- ICT Innovation Group
- Modelling and Simulation (M&S)
  - COTS Simulation Packages (CSPs)
- e-Infrastructures
- e-Infrastructures for M&S
- Conclusions

# ICT Innovation Group, Brunel University

- Technology & knowledge transfer of advanced computing techniques into academia and industry
  - Research, consulting, training and teaching
  - Five academic staff, 3 PDRA + external collaborations
  - 9 PhD Students
  - > £1 million funding
  - Journal of Simulation & ORS Simulation Workshop
- Main areas
  - Modelling and Simulation (Industry & Academia)
  - e-Infrastructure Studies (Europe, Africa)
  - Medical Device Industry Innovation
  - Synthetic and Systems Biology

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# Some outputs

| | |
|---|---|
| Distributed Simulation | ▪ EPSRC Network GROUPSIM<br>▪ CSPI Forum, CSPI PDG<br>▪ IMSS Project (NTU PDCC, Singapore and others) |
| Grid/Cloud Computing | ▪ WINGRID/GridAlliance<br>▪ Industrial projects (Ford, ING, Saker Solutions, Simul8 Corp, WSP, etc.) |
| Research Infrastructure | ▪ BELIEF II<br>▪ ERINA4Africa<br>▪ eI4Africa |
| M&S | ▪ MAP-Guide<br>▪ Cumberland Initiative<br>▪ UK ORS Simulation Study Group, ACM SIGSIM |
| Other | ▪ MATCH Tools and Training<br>▪ Centre for Synthetic and Systems Biology<br>▪ Campus Grid @ Brunel |

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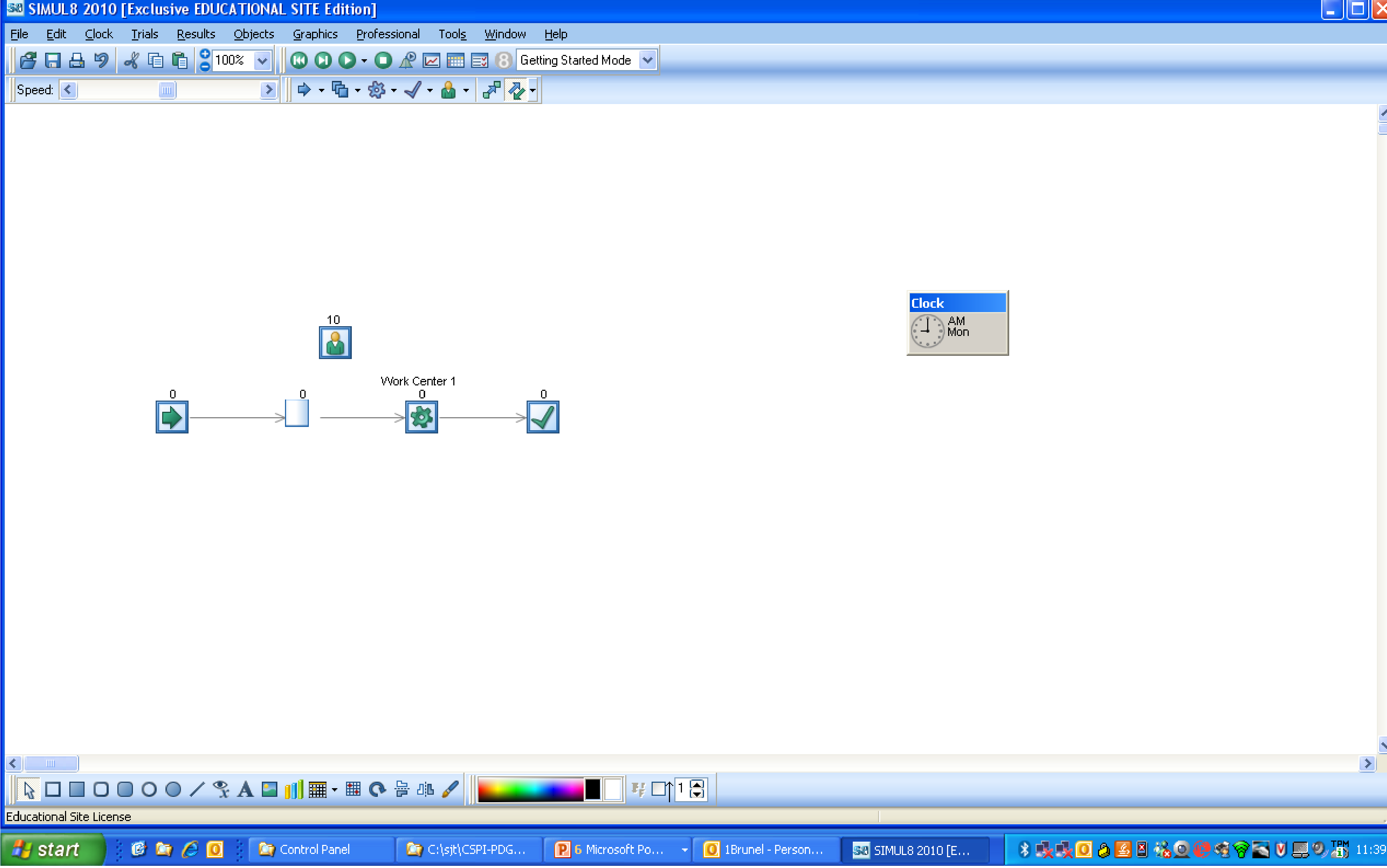
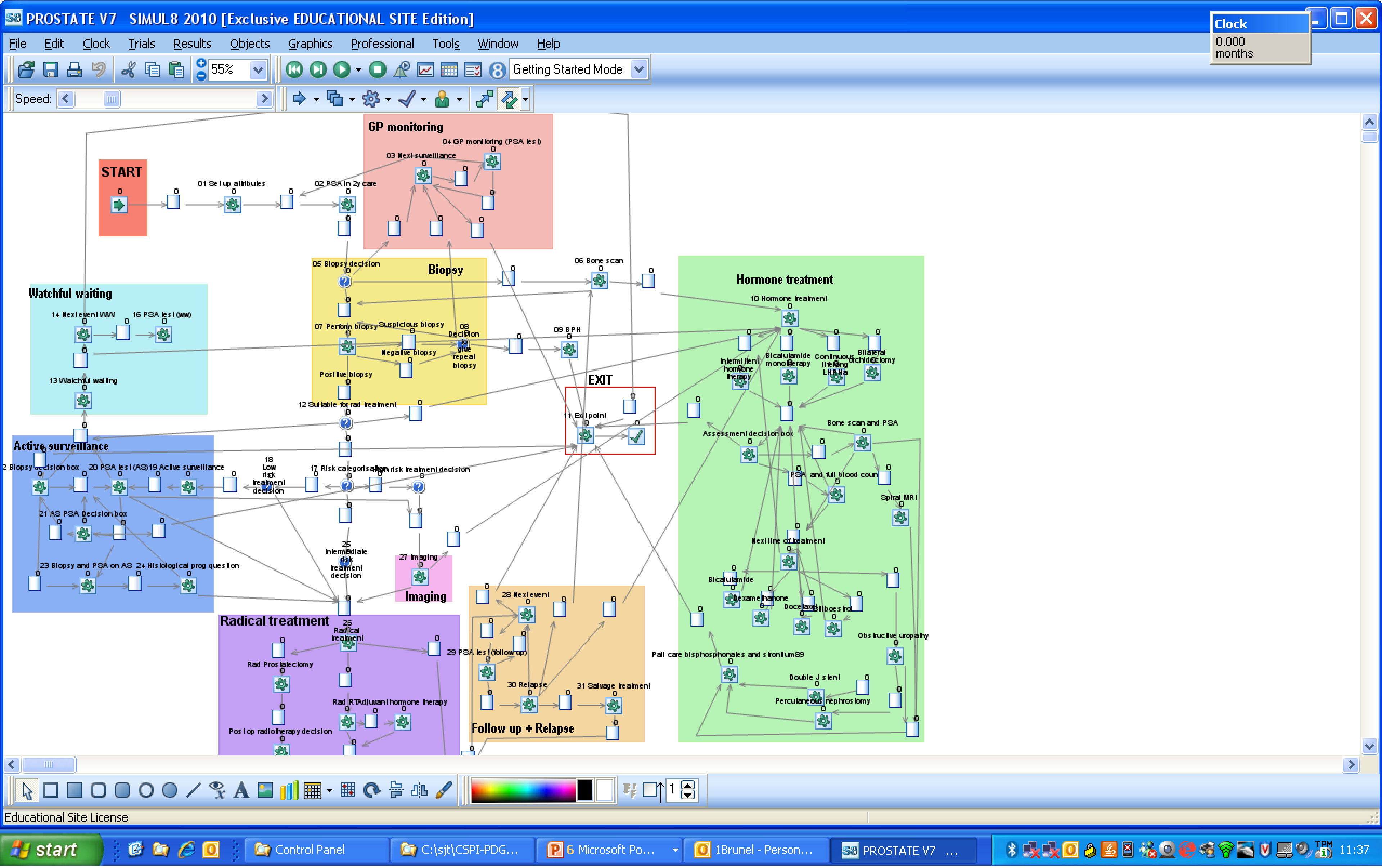
# Modelling & Simulation

- Commerical-off-the-shelf Simulation Packages (CSPs)
  - Arena, AnyLogic, Flexsim, Simio, Simul8, Witness, etc.
  - Widely used to investigate process-based systems in commerce, health, manufacturing, logistics, transportation
  - Discrete-event simulation (some ABS and/or SD)
  - Visual Interactive Modelling (drag and drop)
  - Animated (2D/3D)
  - Methodological support
  - Users tend to be Operational Researchers/Management Scientists




Screenshot of Simul8 (http://www.simul8.com/)




MAP-Guide Project: Prostate Cancer Clinical Pathway v7 in Simul8

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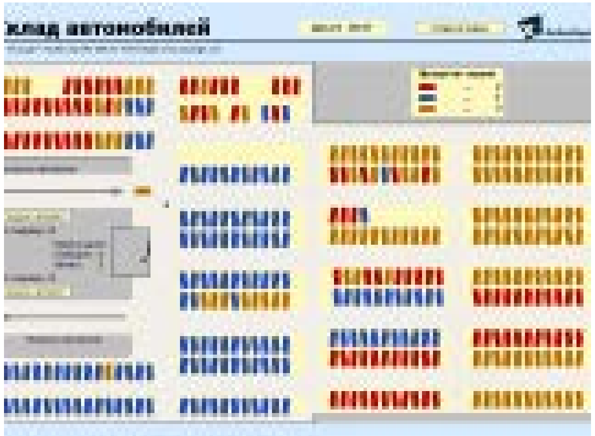
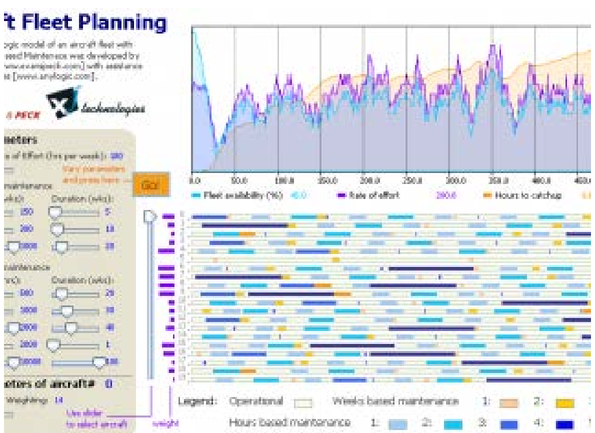
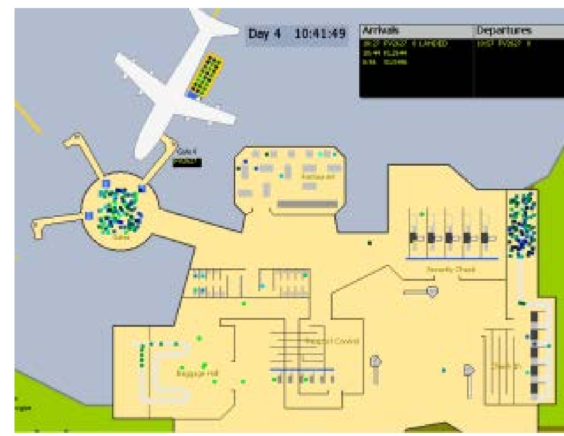
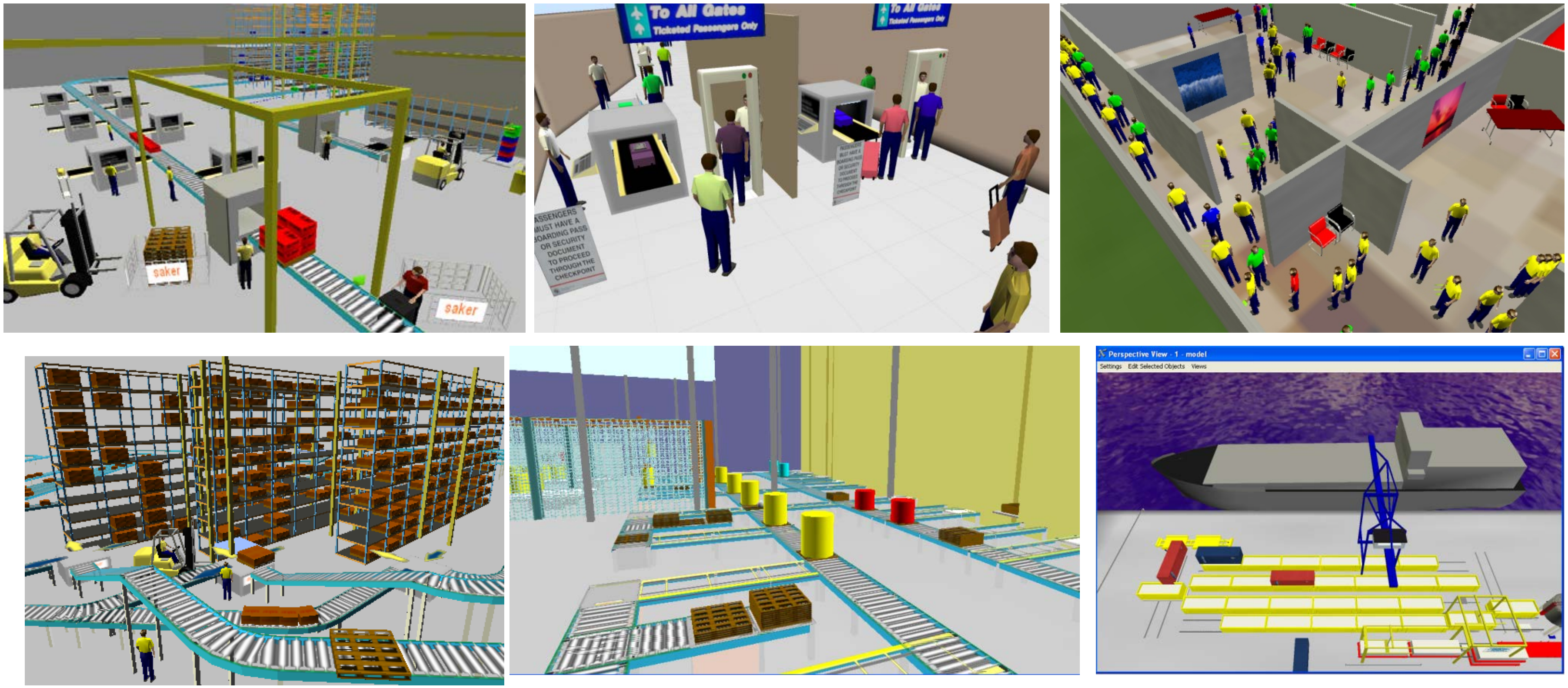







Screenshots from AnyLogic (http://www.xjtek.com/)




Screenshots from Flexsim courtesy of Saker Solutions (http://www.sakersolutions.com/)

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# e-Infrastructures Definition

- An *e-Infrastructure* is
  - an environment where resources—hardware, software, and content—are readily accessible and can be easily shared.
  - It integrates networks, grids, middleware, computational resources, experimental workbenches, data repositories, tools and instruments, and operational support for virtual organizations.
- Supporting worldwide advances in physics (e.g. physics (LHC Grid), biology (biomed) and medicine (Healthgrid))

(https://cordis.europa.eu/fp7/ict/e-infrastructure/home–en.html)

# e-Infrastructures

Global Virtual Research Communities

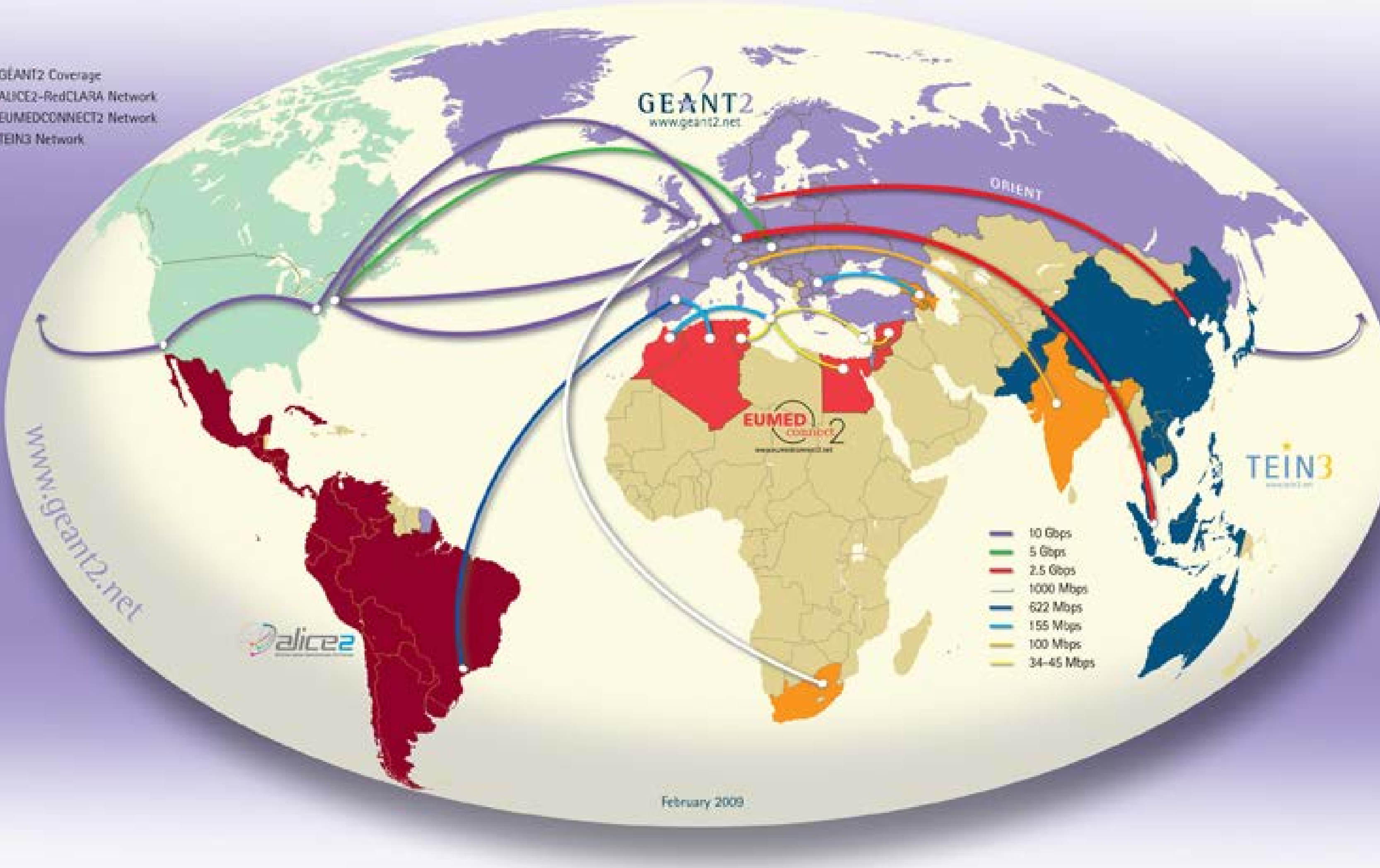
*e-Infrastructure-based Applications*

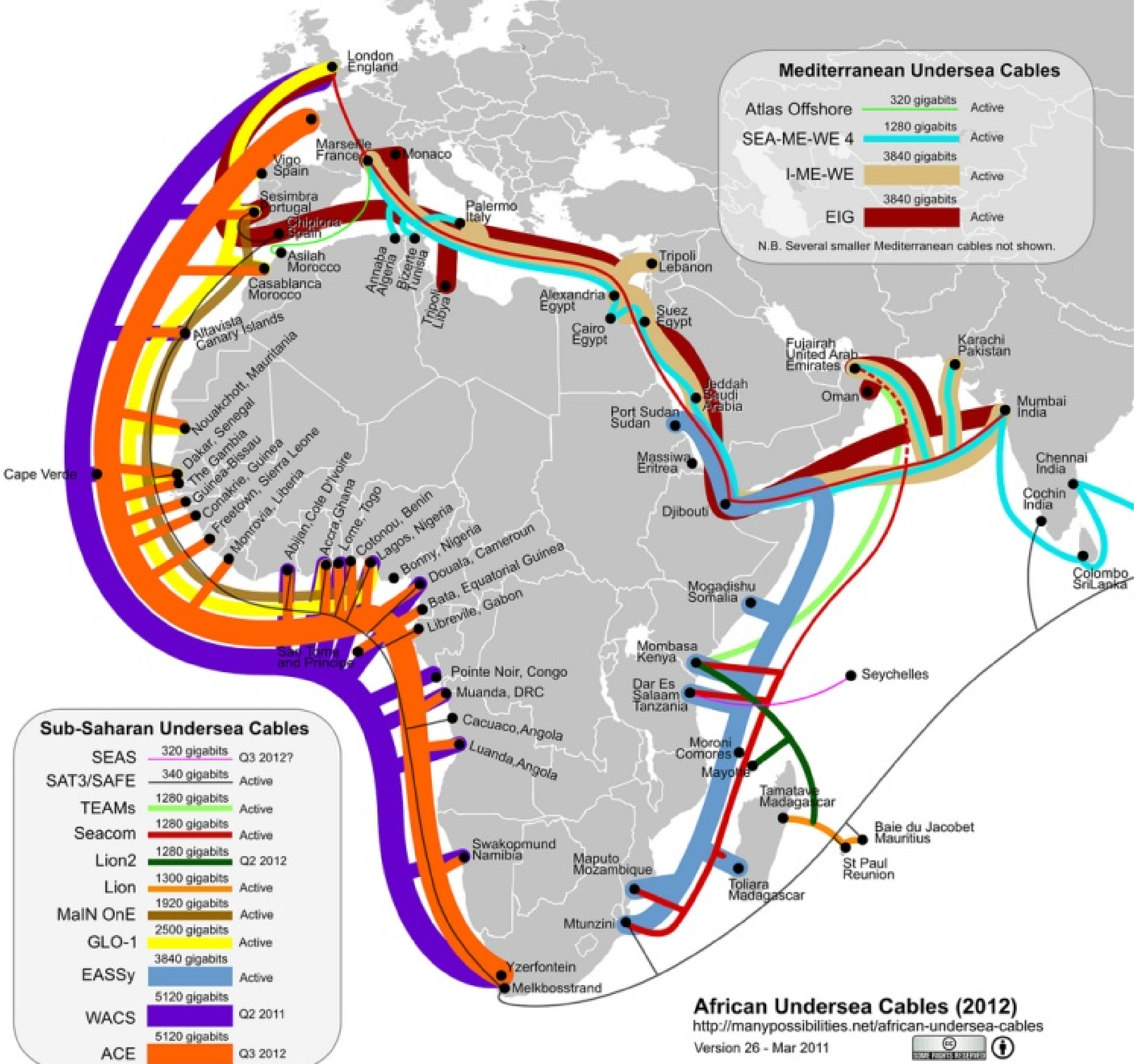
Common middleware support for scientific facilities

e.g. Scientific Digital
Repository Access
Remote instrumentation
Collaboration Support

Distributed & High Performance Computing
(EGI, TeraGrid, PRACE, etc.)

High Performance Network Infrastructure
(GEANT, TEIN, ALICE, etc.)


GÉANT2 Coverage
ALICE2-RedCLARA Network
EUMEDCONNECT2 Network
TEIN3 Network
GEANT2
www.geant2.net
ORIENT
EUMED connect 2
TEIN3
www.geant2.net
alice2
10 Gbps
5 Gbps
2.5 Gbps
1000 Mbps
622 Mbps
155 Mbps
100 Mbps
34-45 Mbps
February 2009


Mediterranean Undersea Cables
Atlas Offshore 320 gigabits Active
SEA-ME-WE 4 1280 gigabits Active
I-ME-WE 3840 gigabits Active
EIG 3840 gigabits Active
N.B. Several smaller Mediterranean cables not shown.
Sub-Saharan Undersea Cables
SEAS 320 gigabits Q3 2012?
SAT3/SAFE 340 gigabits Active
TEAMs 1280 gigabits Active
Seacom 1280 gigabits Active
Lion2 1280 gigabits Q2 2012
Lion 1300 gigabits Active
MaIN OnE 1920 gigabits Active
GLO-1 2500 gigabits Active
EASSy 3840 gigabits Active
WACS 5120 gigabits Q2 2011
ACE 5120 gigabits Q3 2012
London England
Marseille France
Monaco
Vigo Spain
Sesimbra Portugal
Chipiona Spain
Asilah Morocco
Casablanca Morocco
Annaba Algeria
Bizerte Tunisia
Tripoli Libya
Palermo Italy
Tripoli Lebanon
Alexandria Egypt
Cairo Egypt
Suez Egypt
Jeddah Saudi Arabia
Port Sudan Sudan
Massiwa Eritrea
Djibouti
Fujairah United Arab Emirates
Oman
Karachi Pakistan
Mumbai India
Chennai India
Cochin India
Colombo SriLanka
Altavista Canary Islands
Nouakchott, Mauritania
Dakar, Senegal
The Gambia
Guinea-Bissau
Conakrie, Guinea
Freetown, Sierra Leone
Monrovia, Liberia
Cape Verde
Abijan, Cote D'Ivoire
Accra, Ghana
Lome, Togo
Cotonou, Benin
Lagos, Nigeria
Bonny, Nigeria
Douala, Cameroun
Bata, Equatorial Guinea
Librevile, Gabon
Sao Tome and Principe
Pointe Noir, Congo
Muanda, DRC
Cacuaco, Angola
Luanda, Angola
Swakopmund Namibia
Yzerfontein
Melkbosstrand
Mogadishu Somalia
Mombasa Kenya
Dar Es Salaam Tanzania
Seychelles
Moroni Comores
Mayotte
Tamatave Madagascar
Baie du Jacobet Mauritius
St Paul Reunion
Toliara Madagascar
Maputo Mozambique
Mtunzini
African Undersea Cables (2012)
http://manypossibilities.net/african-undersea-cables
Version 26 - Mar 2011

# Key Issues (UK)

- Network
  - The supra-exponential growth in data and the need to share this data for effective collaboration. Securing and expanding this is a priority.
- Software People and Skills
  - Robust and usable software at every level of the e-Infrastructure supported by skilled software engineers and developers.
- Compute
  - On-going national need for robust computing infrastructure to facilitate the ongoing need for to run simulations. Cloud (e.g. Amazon EC2) emerging.
- Data
  - Expanding data deluge. (Need for curation, management and certification).

e-Infrastructure Advisory Group (2011), Report of the e-Infrastructure Advisory Group, Research Councils UK

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# e-Infrastructure Involvement/Influence

- Bringing Europe's eLectronic Infrastructures to Expanding Frontiers (BELIEF 1 & 2) (Europe, Latin America & India)
- Organisation of e-Infrastructure Concertation events (Europe)
- Exploiting Research Infrastructures potential for Boosting Research and Innovation in Africa (ERINA4Africa) (Europe & Africa)
- eI4Africa (Europe & Africa)
- European Desktop Grid Initiative Subcontract

# e-Infrastructures for M&S

- An *e-Infrastructure for M&S* (in the context of this talk) is
  - an environment where resources — **COTS simulation packages and ancillary software (e.g. Excel), models, data, etc.** — are readily accessible and can be easily shared **and/or interoperated**
  - It integrates networks, grids, middleware, computational resources, data repositories, and software tools within (virtual) organizational boundaries
- What could be the specific benefits?

# e-Infrastructures for M&S – Benefits?

- Collaborative Support
  - Save project time and costs by remote collaboration
- High Speed Experimentation
  - Reduce experimentation time and/or increase depth of analysis
- Simulation Interoperability/Distributed Simulation
  - Reduce experimentation time and/or increased analysis, facilitate distributed model development, overcome large distributed model problems
- Data (Artefact) Management
  - Project cost reduction by better management of all simulation project artefacts, integration with other projects, cheaper model development through reuse

# e-Infrastructures for M&S

## Collaborative Support

- Groupware
- Plenty of off-the-shelf software (Messenger, Skype, GotoMeeting, etc.)
- Application sharing
- On-line training opportunities
- Cannot replace face-to-face meetings but can certainly reduce model development time (less time travelling!)
- BUT!
  - Some practitioners unaware that groupware exists!

# e-Infrastructures for M&S
# High Speed Experimentation

- COTS Simulation Packages
  - Nearly all run under Windows
  - Must be installed
  - Access to local installed data sources (databases, spreadsheets, etc.)
  - Are licensed (typically by copy)
  - Do not have direct Grid/Cloud Computing support
  - Model runtimes seconds to hours

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# e-Infrastructures for M&S
# High Speed Experimentation

- Grid and/or Cloud Computing
  - Must be easy to implement and support
  - M&S is costly! Must be a clear business case for Grid investment
  - Users will have OR/MS skill set - must be deployed in their 'world' (experimentation managers)
  - Institutional IT management plays a key role and must be on board

# Desktop Grid Computing and M&S

- Ford
  - WINGRID/WITNESS
- ING
  - WINGRID/EXCEL
- GRIDALLIANCE
  - WINGRID/SIMUL8
- Systems Biology
  - CONDOR/SIMAP
  - SZDG/SIMAP
- Saker Solutions
  - SAKERGRID/FLEXSIM
- SIMUL8
  - SZDG/SIMUL8 & EXCEL

**2008+ Literature**

**2008**
Mustafee and Taylor (2008) *SW '08*, Mustafee and Taylor (2008) *WSC 2008*

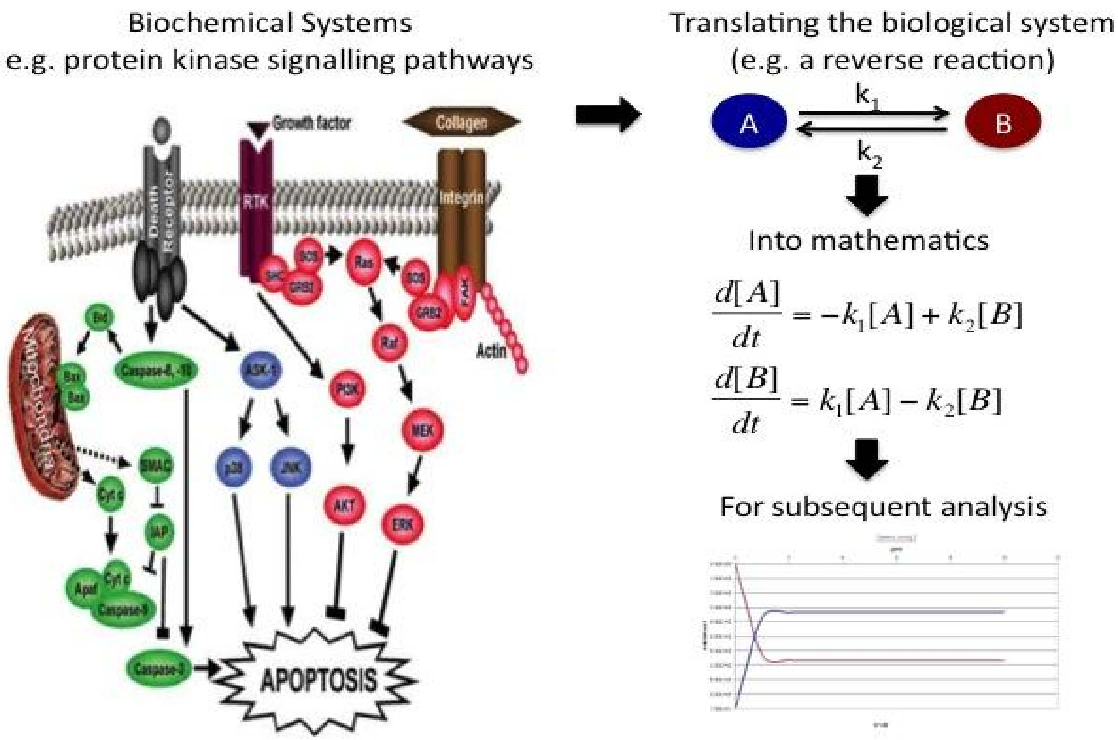
**2009**
Wang, et al. (2009) *AHM 2009*, Mustafee and Taylor (2009) *Concurrency and Computation: Practice and Experience*, Mustafee and Taylor (2009) *Grid Technology for Maximizing Collaborative Decision Management and Support*

**2010**
Taylor, et al. (2010) *WSC 2010*, Mustafee and Taylor (2010) *WSC 2010*, Mustafee and Taylor (2010) *SW '10*, Wood, C., et al. (2010) *SW '10*

**2011**
Kite, et al. (2011) *WSC 2011*

**2012**
Taylor, et al. (2023) *SW'12*

# Systems Biology




Orton, et al. (2005)
*Biochem J*

Liu, et al. (2008)
*Studies in Health Technologies and Informatics*

SIMAP Systems Biology Simulation Tool (Glasgow/Brunel)

Uses SBMLODEsolver (SOSLib) to compute the concentrations of species over time.

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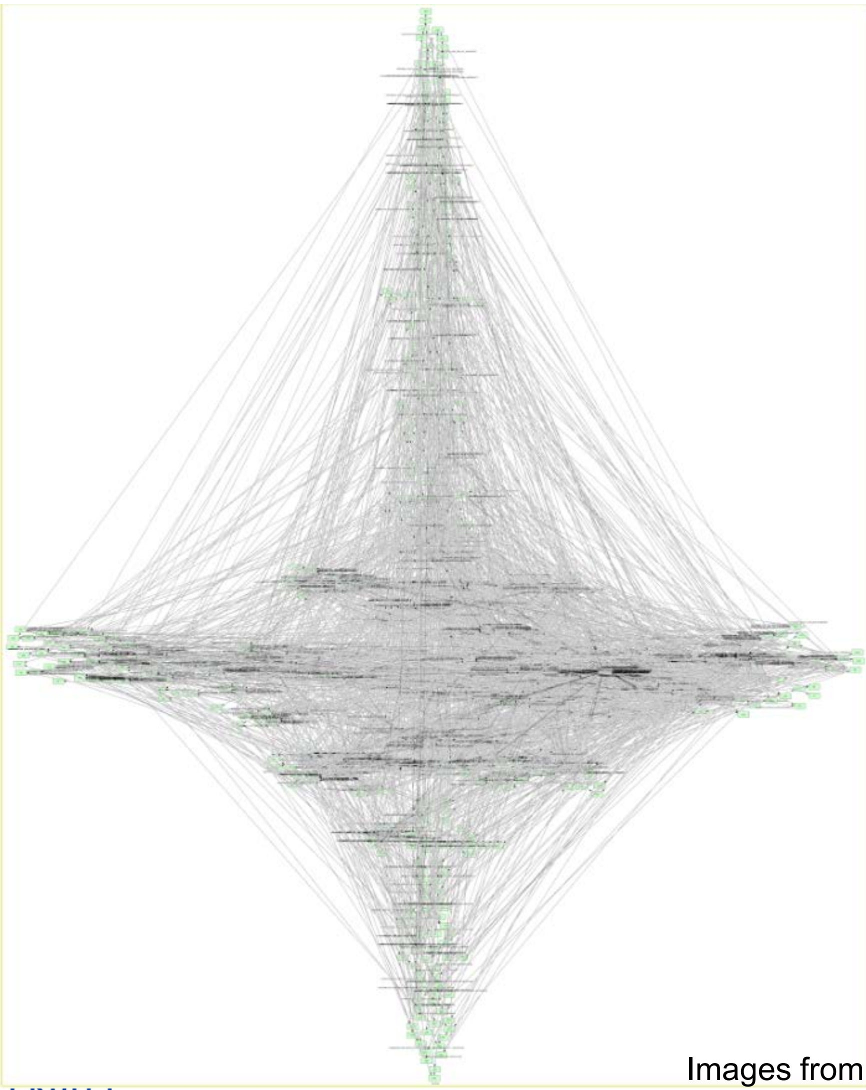
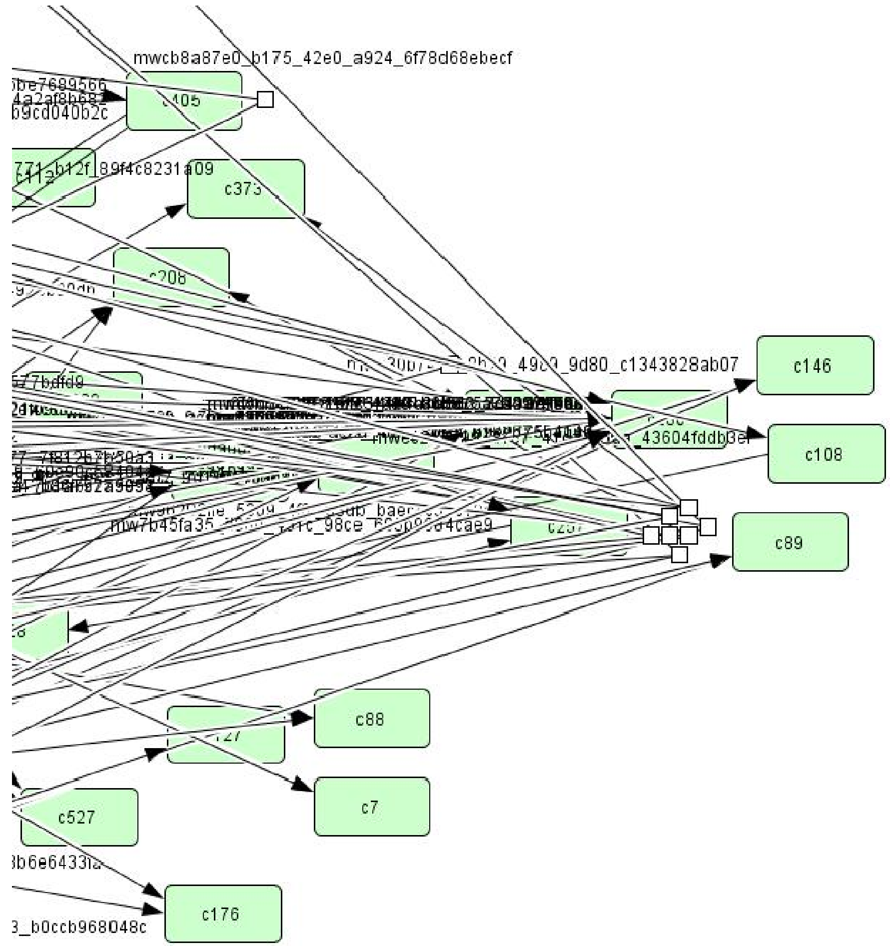
- Models are specified by Systems Biology Mark up Language (SBML)


```xml
- <species id="mw132274B8_625A_4C28_8B55_2B0D5480F46A" name="c558" compartment="mwE8BCI
    initialAmount="0">
    <notes>(EGF:ErbB1:ATP::EGF:ErbB1_h:Inh)-HalfActive</notes>
    <annotation>plasma membrane</annotation>
  </species>
</listOfSpecies>
- <listOfParameters>
  <parameter id="mw8b4a0e01_6b31_4b99_93ac_0a1df7ad377b" name="kd1" value="0.0033" />
  <parameter id="mw10be3c14_8b28_4a67_b3e6_5b2987d003d0" name="k1c" value="800" />
  <parameter id="mw817a95bd_e5c8_4a5c_b088_01810dafd40c" name="kd1c" value="1" />
  <parameter id="mw611b22c9_7afd_4364_98d7_fb6ed1ce06b8" name="kd1d" value="0.1" />
```

# MAPK model (732 species, ~ 244 parameters)






Images from Celldesigner

# Grid Computing & Systems Biology

- Two kinds of analysis that can benefit from grid computing
  - **Parameter scanning** and Parameter estimation
- Parameter scanning changes kinetic rates and creating new models the number of models can grow very fast
- ‘Typical’ model runs at around 20-30s (Contemporary PC)
  - 2 parameters over 10 values @ = ~11 hours
  - 3 parameters over 10 values @ =  ~3 months

# Desktop Grid Architecture

- Previous studies on CONDOR
  - Wang, et al. (2009) *AHM 2009*
- Recent studies on SZTAKI Desktop Grid (SZDG)
  - Based on volunteer computing adaptation based on Berkley Open Infrastructure for Network Computing (BOINC)
  - EDGeS & EDGI projects
    - www.edges-project.eu, www.edgi-project.eu
  - Any application can run, does not use credits
  - Westminster Local Desktop Grid (WLDG)
    - An implementation of SZDG
    - 1500 PCs, four different sites

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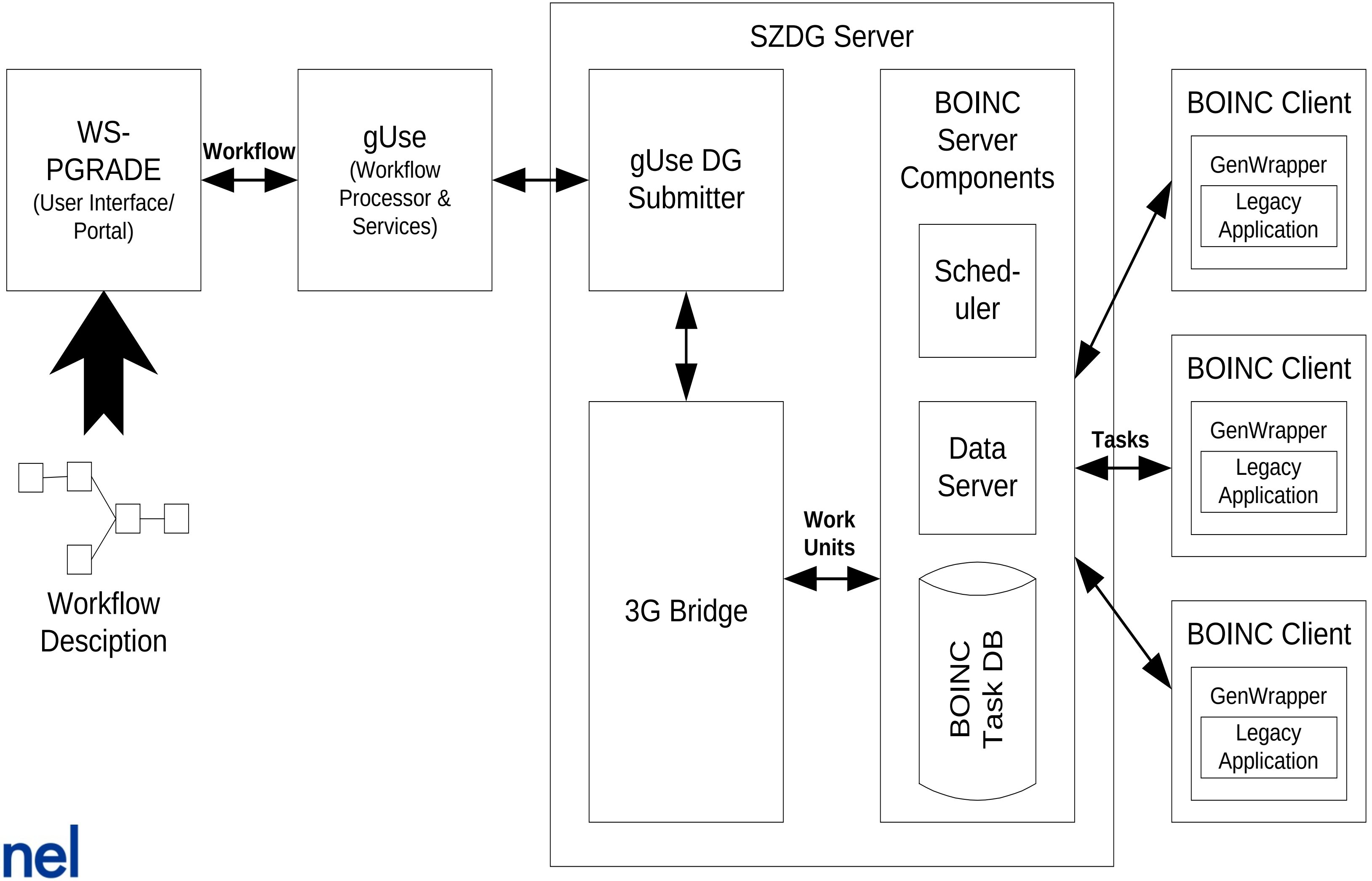
# BOINC

| Projects | Users | last day | Hosts | last day | Teams | last day | Countries | last day | Total credit | last day |
|---|---|---|---|---|---|---|---|---|---|---|
| **BOINC combined** | 2,080,715 | +518 | 5,894,410 | +1,903 | 89,775 | +8 | 272 | 0 | 362,133,002,359 | +921,651,669 |
| MilkyWay@home | 82,959 | +149 | 159,949 | +269 | 2,321 | +1 | 188 | +1 | 61,252,351,250 | +218,560,609 |
| DNETC@HOME | 3,503 | +14 | 9,262 | +45 | 424 | +3 | 105 | 0 | 30,008,025,659 | +173,066,153 |
| Collatz Conjecture | 15,511 | +39 | 33,842 | +80 | 919 | +1 | 133 | 0 | 41,764,474,956 | +141,452,933 |
| SETI@Home | 1,137,030 | +117 | 2,762,616 | +297 | 58,341 | +2 | 234 | 0 | 86,481,304,588 | +20,396,572 |
| World Community Grid | 319,238 | +130 | 1,085,581 | +669 | 18,463 | +5 | 219 | 0 | 33,869,775,598 | +47,131,133 |
| AQUA@home | 20,158 | +41 | 38,150 | +79 | 879 | +1 | 145 | 0 | 10,656,666,052 | +40,541,195 |
| Einstein@Home | 283,397 | +89 | 1,932,363 | +992 | 9,594 | 0 | 216 | 0 | 25,892,830,400 | +34,183,074 |
| PrimeGrid | 36,018 | +53 | 111,997 | +123 | 1,874 | +4 | 174 | 0 | 6,122,272,891 | +154,725,985 |
| GPUGRID | 10,917 | +15 | 19,318 | +24 | 779 | 0 | 114 | 0 | 13,427,792,182 | +30,354,391 |
| Climate Prediction | 239,960 | +95 | 475,773 | +206 | 7,253 | +1 | 217 | 0 | 13,979,786,946 | +17,161,536 |
| Rosetta@Home | 305,938 | +91 | 948,159 | +292 | 9,088 | 0 | 222 | 0 | 12,438,794,431 | +13,422,723 |
| QMC@Home | 44,280 | +10 | 109,359 | +42 | 2,018 | 0 | 174 | 0 | 3,460,086,620 | +4,149,686 |
| Docking@Home | 21,030 | +20 | 54,041 | +46 | 793 | 0 | 128 | 0 | 1,427,858,985 | +3,642,907 |
| FreeHAL | 9,853 | +21 | 37,866 | +54 | 561 | 0 | 116 | 0 | 2,262,737,192 | +3,883,096 |
| ABC@home | 40,346 | +48 | 91,351 | +62 | 1,439 | -1 | 173 | 0 | 2,763,248,315 | +2,107,687 |

- 1 Gigaflop machine running for a day ~ 200 credits
- => BOINC combined ~ 4.5 Million Gigaflops/day

# SZTAKI Desktop Grid (SZDG)



# University of Westminster Local DG

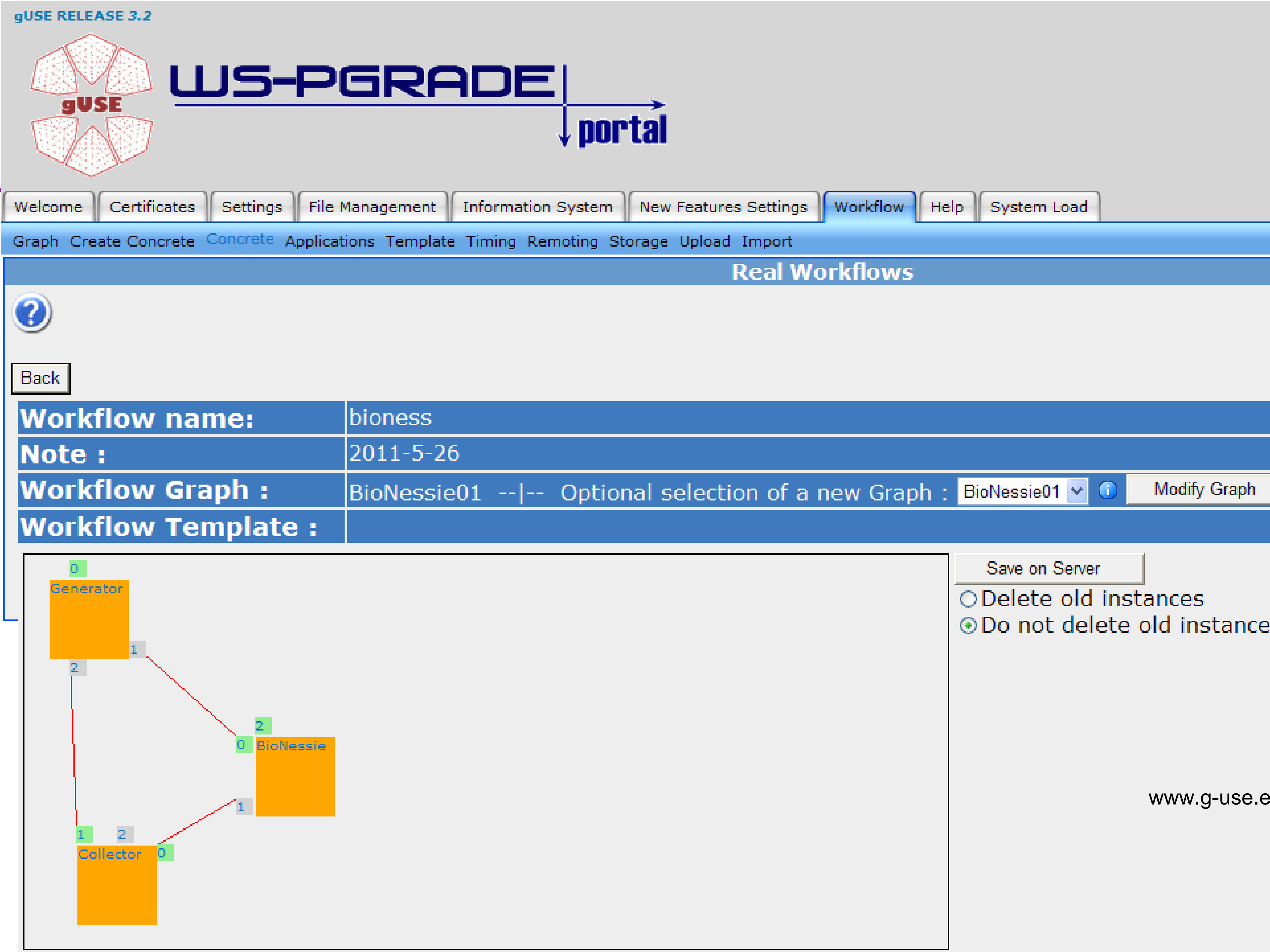
Over 1500 Windows PCs from 6 different campuses


| | |
|---|---|
| 1 New Cavendish St | 576 nodes |
| 2 Marylebone | 559 nodes |
| 3 Regent Street | 395 nodes |
| 4 Wells Street | 31 nodes |
| 5 Little Titchfield St | 66 nodes |
| 6 Harrow Campus | 254 nodes |

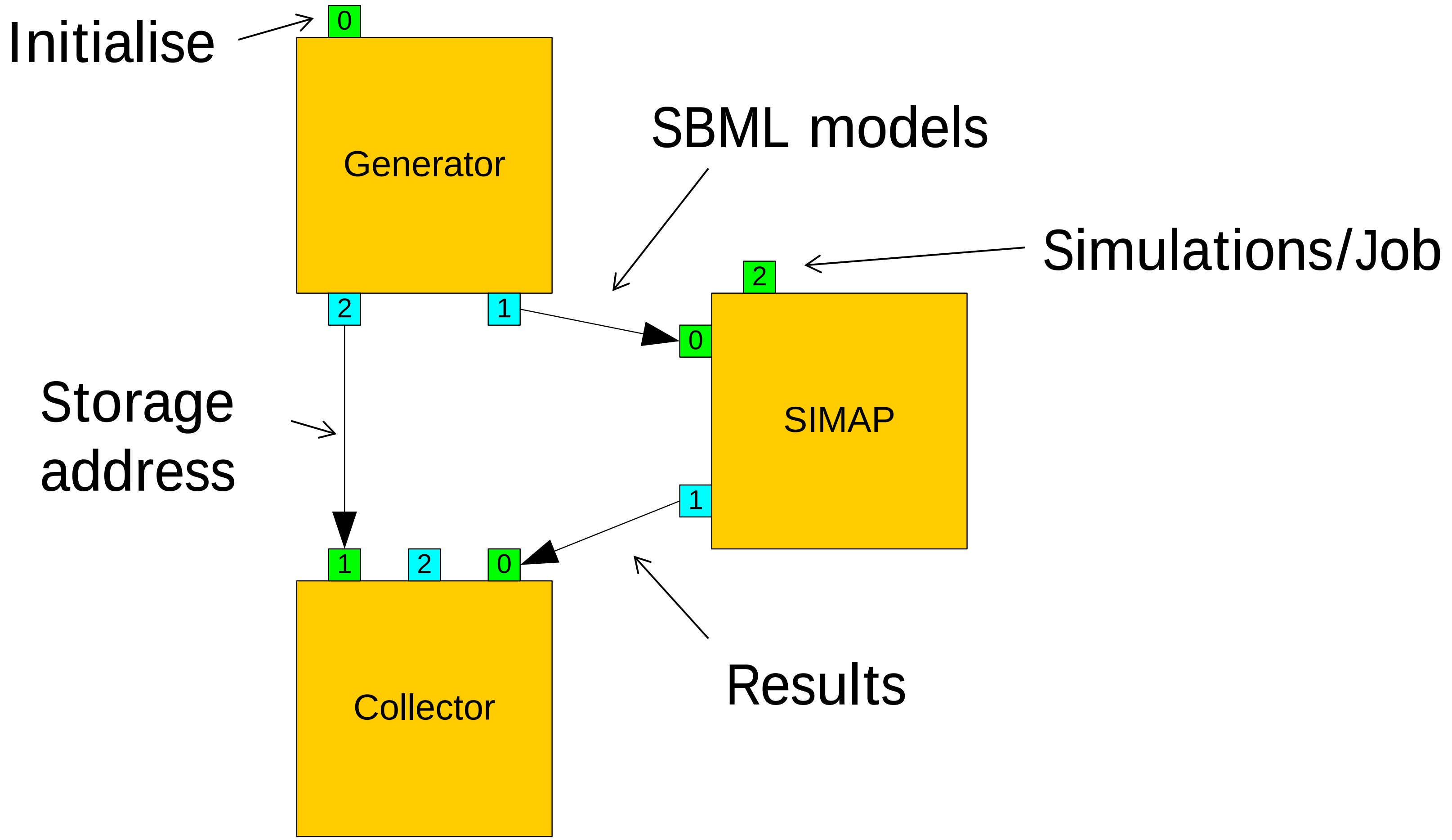
Courtesy of Centre for Parallel Computing, University of Westminster

**Lifecycle of a DG node:**

1. PCs basically used by students/staff
2. If unused, switch to Desktop Grid mode
3. No more work from DG server -> shutdown (green solution)


gUSE RELEASE 3.2
gUSE
WS-PGRADE
portal
Welcome
Certificates
Settings
File Management
Information System
New Features Settings
Workflow
Help
System Load
Graph
Create Concrete
Concrete
Applications
Template
Timing
Remoting
Storage
Upload
Import
Real Workflows
Back
Workflow name:
bioness
Note :
2011-5-26
Workflow Graph :
BioNessie01 --|-- Optional selection of a new Graph :
BioNessie01
Modify Graph
Workflow Template :
Save on Server
Delete old instances
Do not delete old instance
Generator
BioNessie
Collector
www.g-use.e

# WS-PGRADE Portal Workflow



# Job (work unit) Description

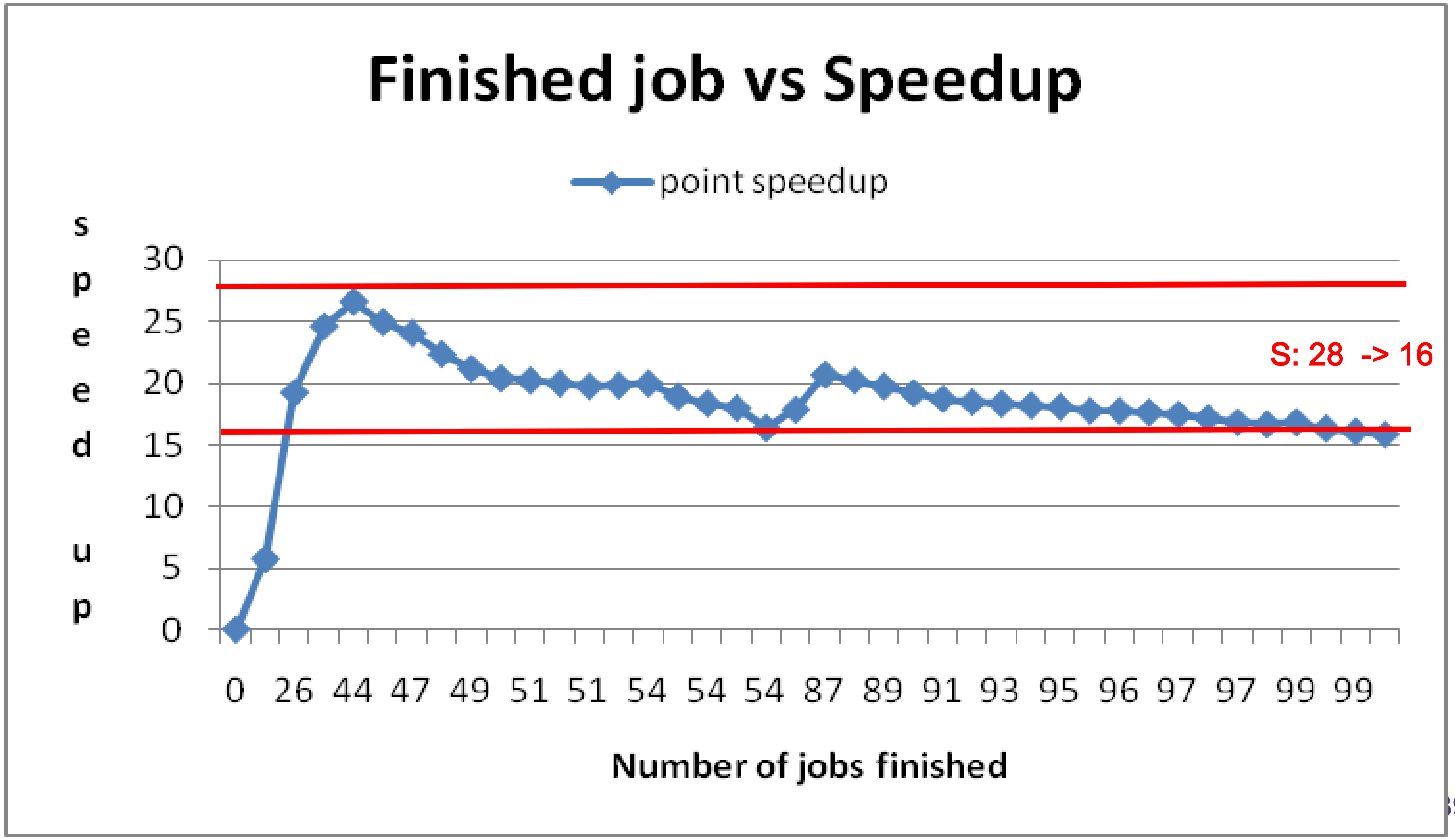
- Inputs
  - SBML model
  - Script file
  - SBMLOdesolver
  - Size: ~2 MB.
- Output
  - Zip file contains results for all jobs
  - Size: ~1.5 MB.

# Speedup vs Job Completion

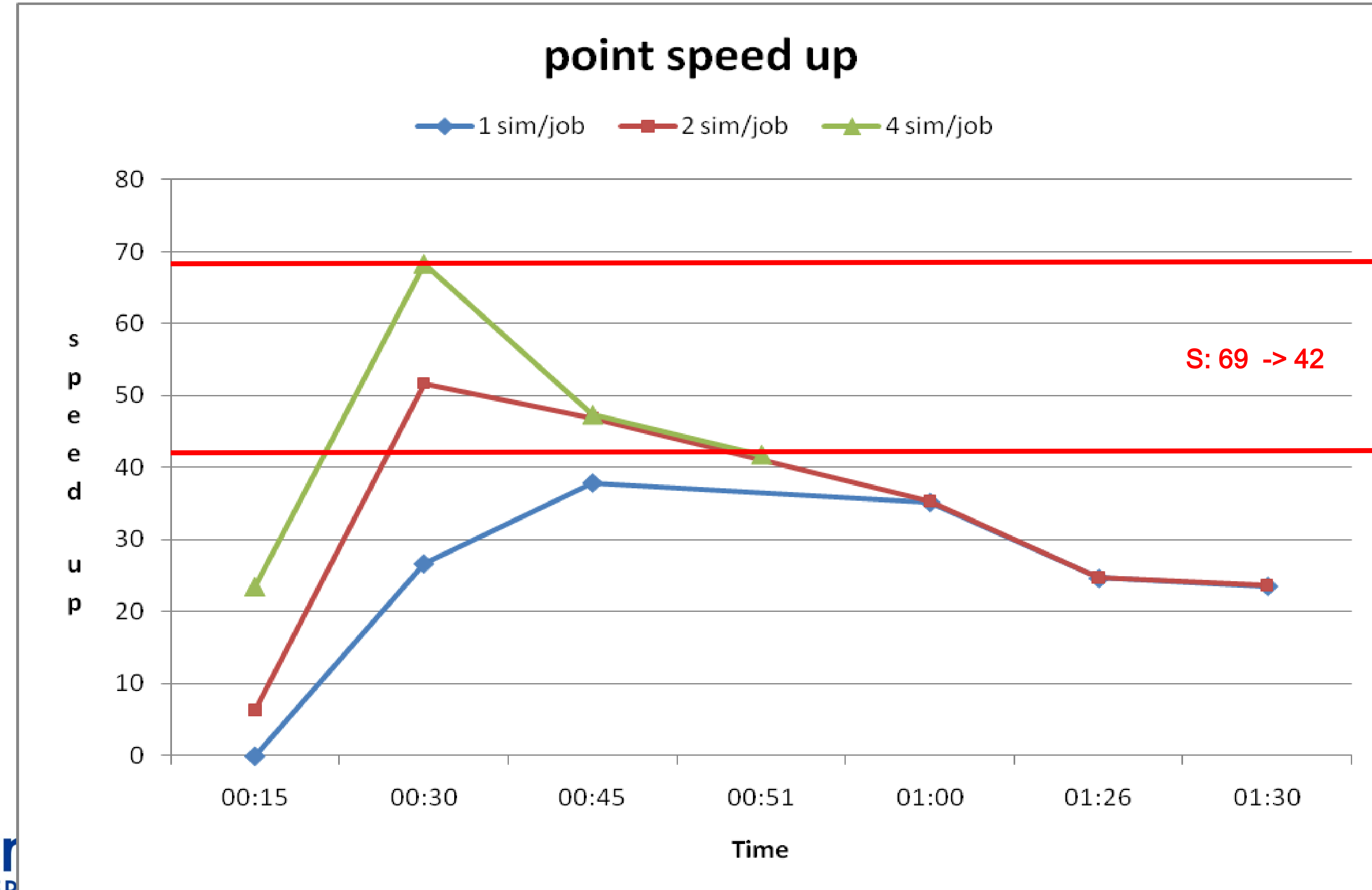
100 jobs, 100 simulations per job

30 min to complete ~50% of jobs, 2h 30 min to complete other ~50%

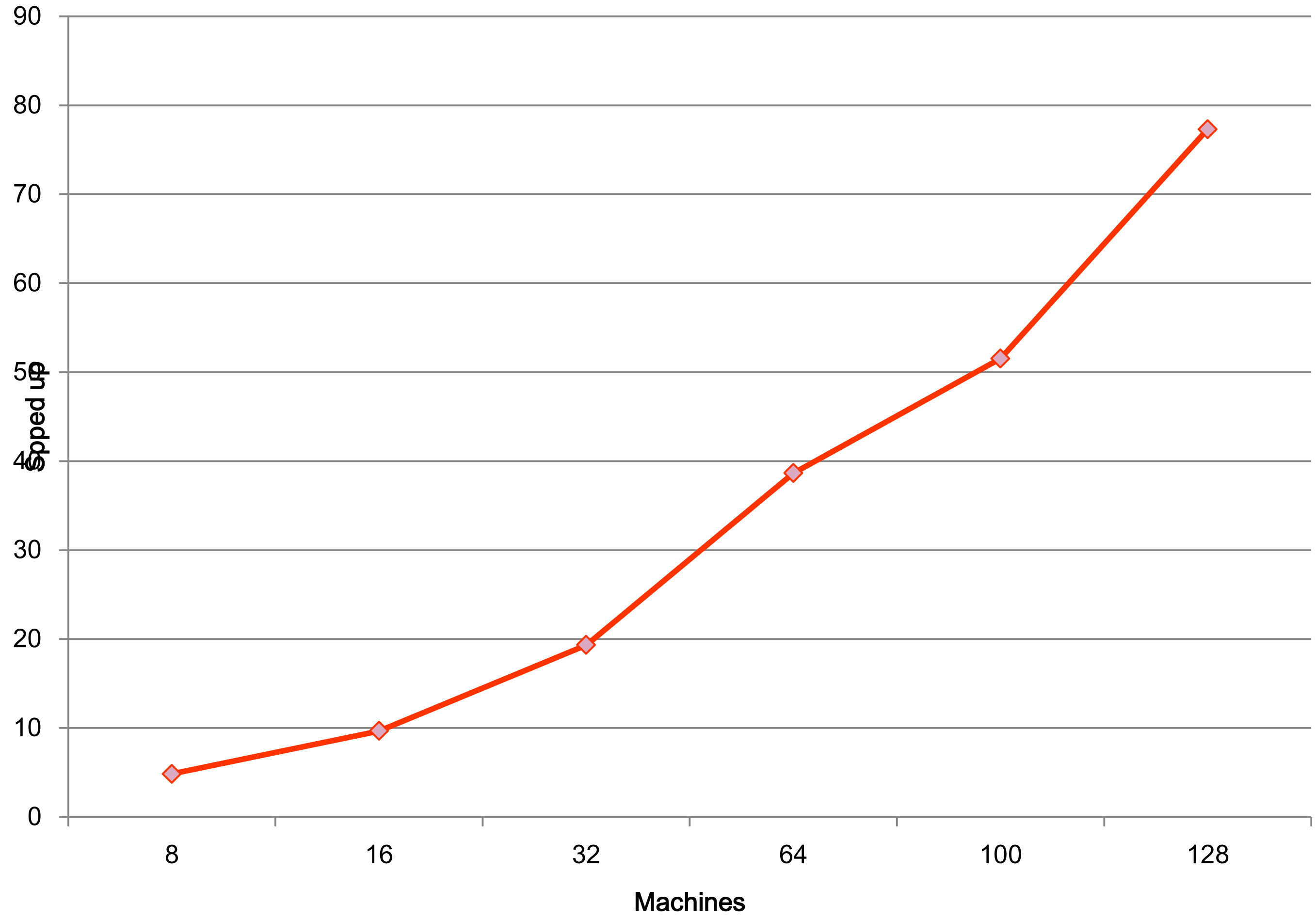
Unknown number of PCs



# Speedup vs Job Completion

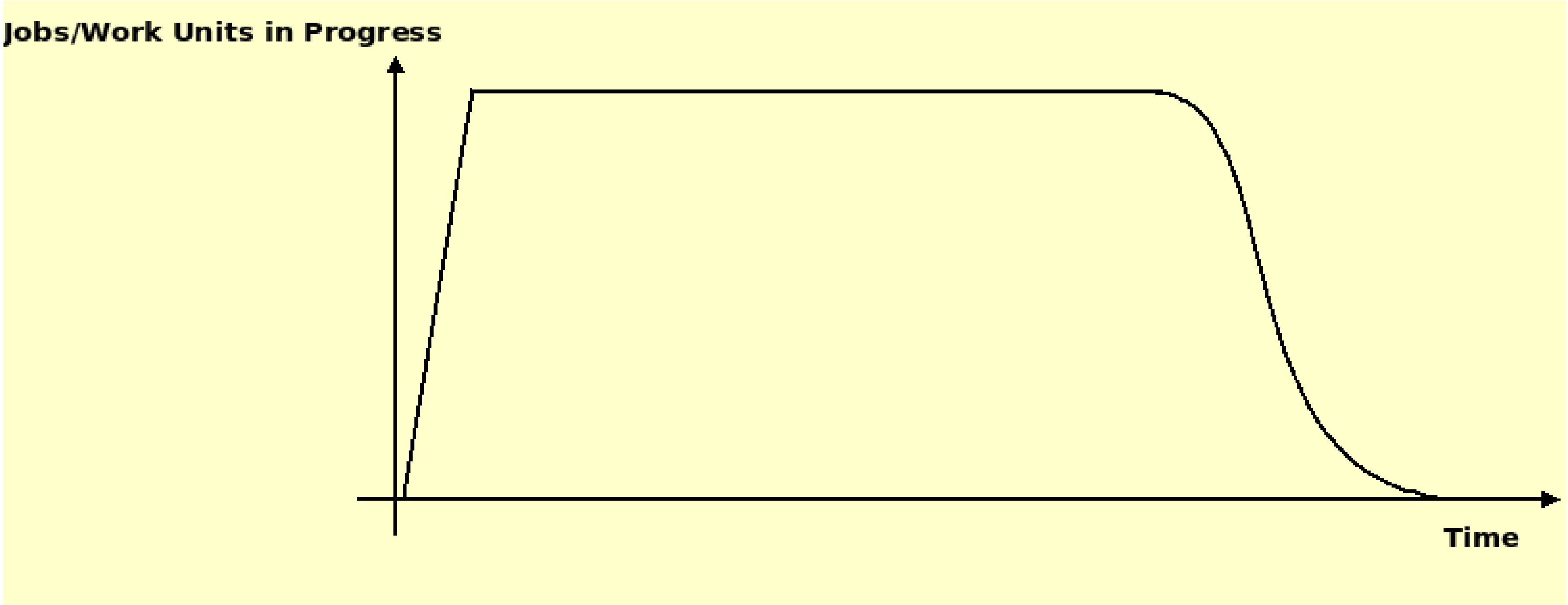


# CONDOR Speedup (8 sims/job)



# Volunteer Computing

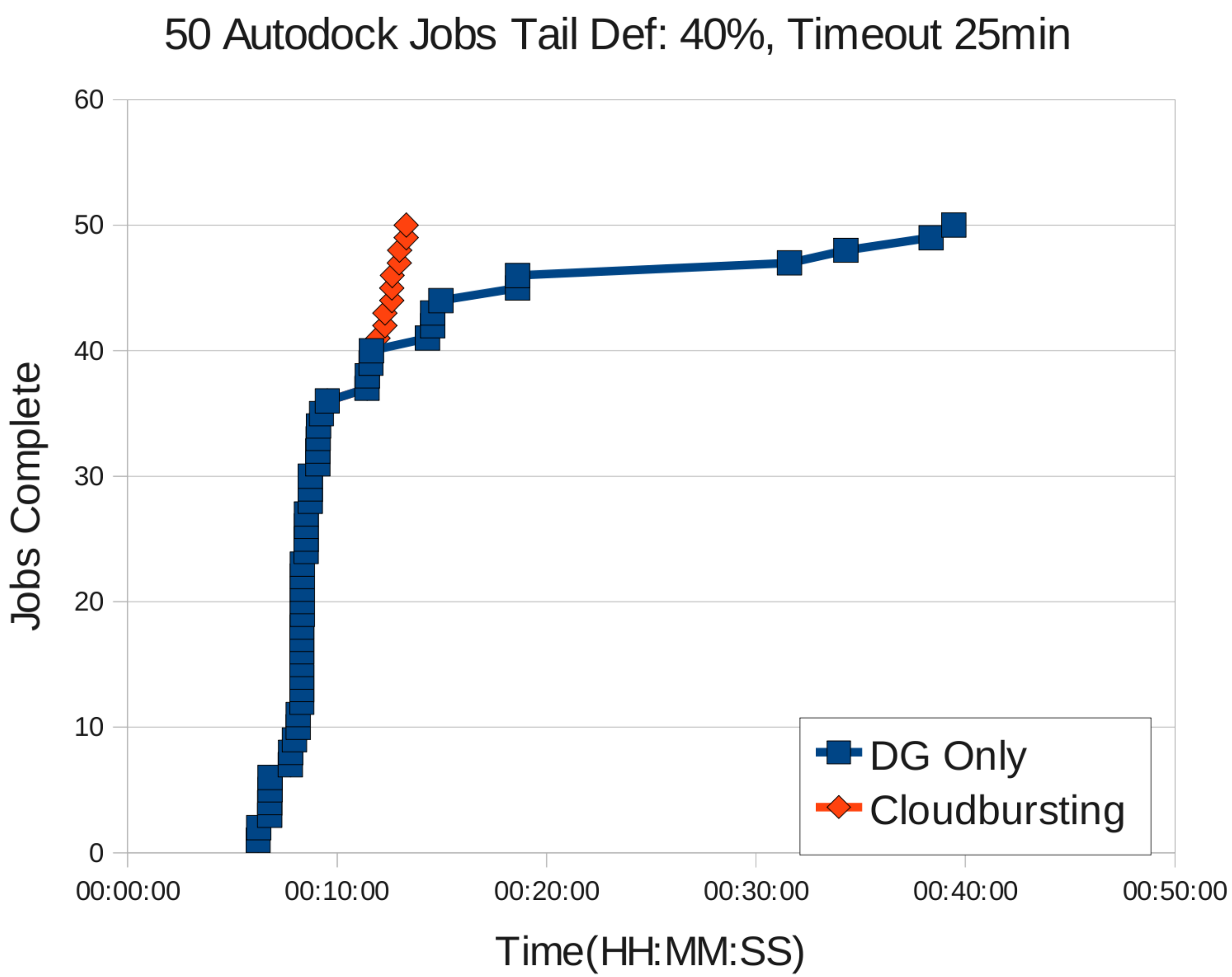
## Tail Problem



# Cloudbursting

- Augment the DG infrastructure with virtual cloud resources
- Design a cloud resource scheduler that tackles the tail problem

# Cloudbursting: Indicative Results




*With thanks toCentre for Parallel Computing, 2011*

# Summary (DG/Systems Biology)

- Some success but limited variable speedup
- More experimentation
  - Cloudbursting
- Possible standardised approach
  - Several SZDG implementations/applications can run on any SZDG platform
  - Links to EGI systems via 3G Bridge
- Portal/job submission technology
  - Developing G-Use Portal for SIMAP

# SAKERGRID

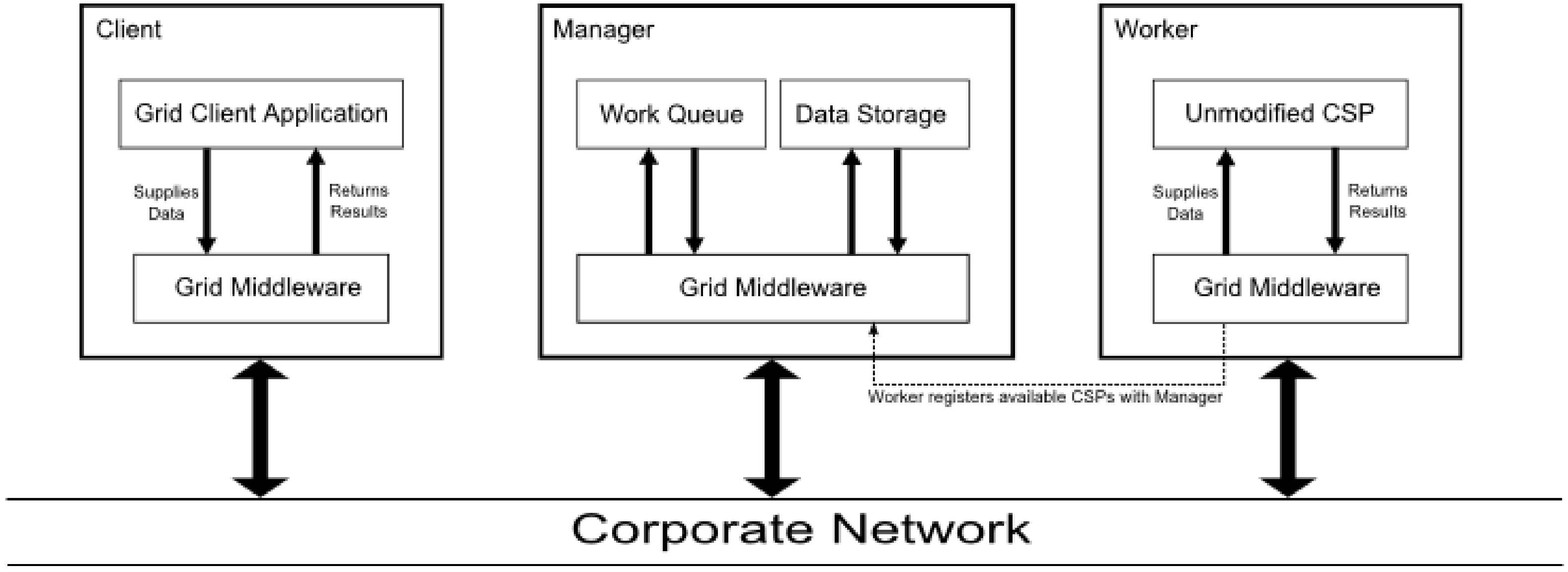
- Saker Solutions identified a need to radically reduce the time taken to produce results from a simulation project.
- Joint research Project with Brunel University during 2007-9
- Culminated in the development of SAKERGRID
- 1st Large Scale Client Implementation at Sellafield Ltd (BNFL) 2010

Taylor, et al. (2010) *WSC 2010*, Wood, et al. (2010) *SW '10*, Kite, et al. (2011) *WSC 2011*

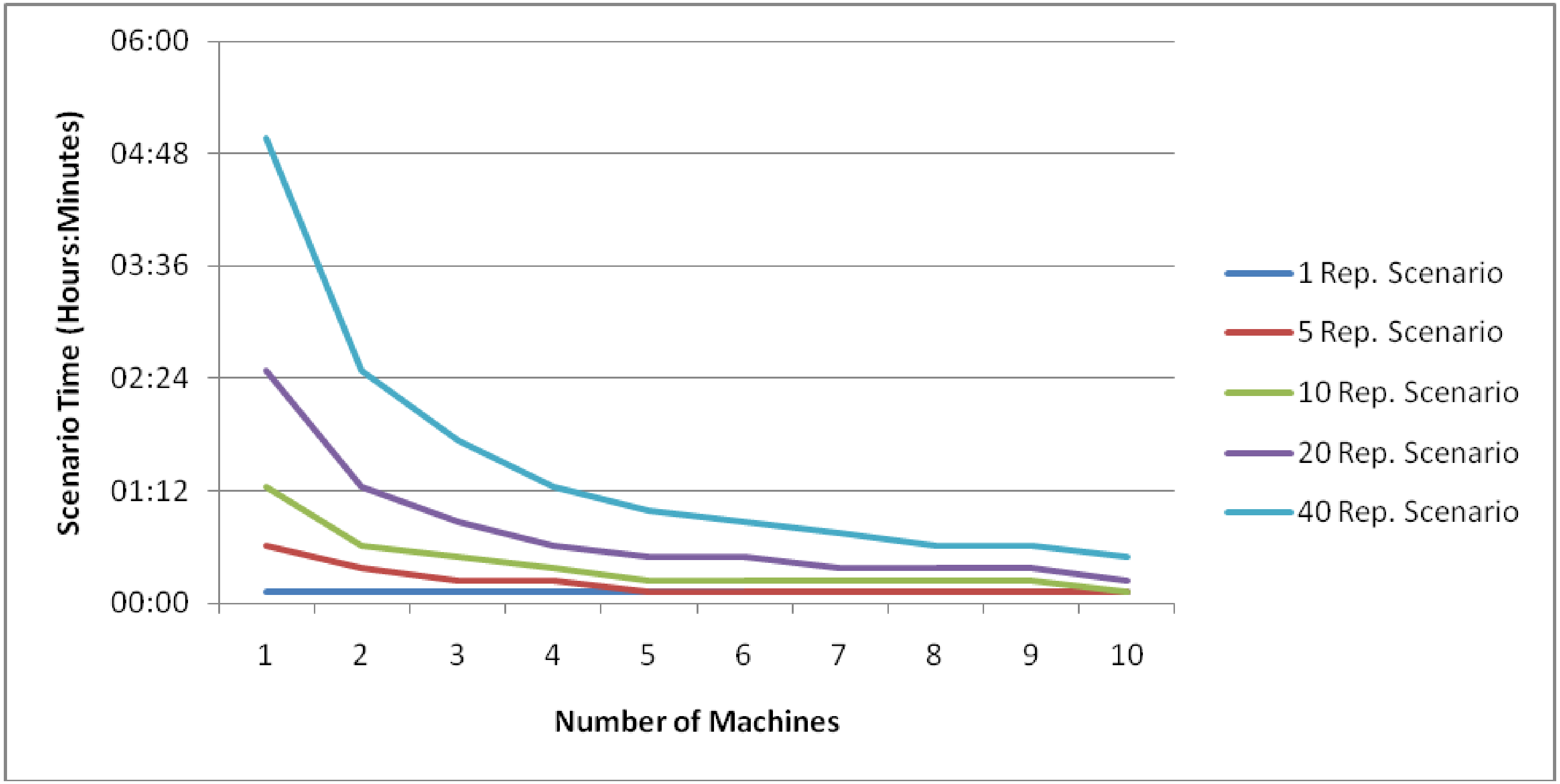
# Development Issues

- Testing existing approaches against possible client sites led to development of bespoke Grid implementation
  - Potential wide range of implementation challenges
  - Develop well-understood, in-house technology
- CSP
  - Initially Flexsim
- Integration with Saker's Scenario Manager
  - Manager/'Portal'
- Assumes
  - CSP/Models/data available locally at worker
  - Client has multiple licences

# SAKERGRID Architecture



# Conventional Speedup



# Sellafield Ltd UK & Flexsim

- Sellafield Ltd is responsible for safely delivering decommissioning, reprocessing, nuclear waste management and fuel manufacturing activities
- Sellafield Ltd have a network with 22 Flexsim Licences based over 3 sites
- There are up to a dozen client machines that need to submit jobs to the manager
- Workers each hold a Flexsim Licence.
  - They may sit on the same machine as the client.
  - They may sit on a series of dedicated multicore servers running VMware to host multiple Virtual Machine instances.
- Models have runtimes of between 10 mins and 12 hours per replication
- Models are all Flexsim models but using different versions of the software and different libraries

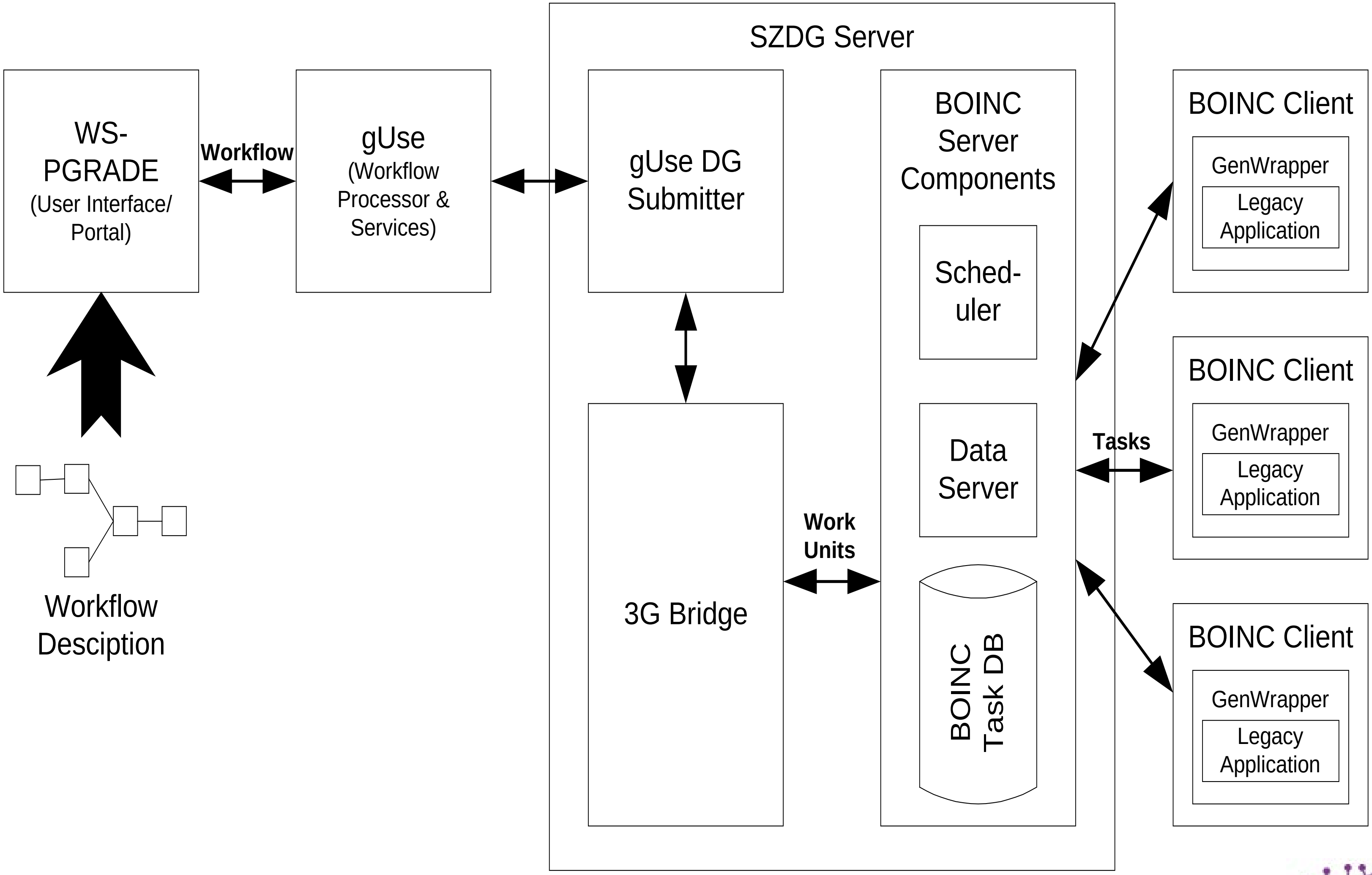
# Sellafield Ltd & SAKERGRID

- User conflict
  - Running Grid in the background is not always desirable. Some models have a requirement for 2GB of Memory
- Network infrastructure
  - Restricted Shared folders on machines
- Inter-Site networking
  - Frequent disconnects , sometimes as frequent as every 30 mins.
- Security
  - Cannot leave a model and results together on a machine – delete when finished
- SAKERGRID successfully modified to account for these issues

# Summary (SAKERGRID)

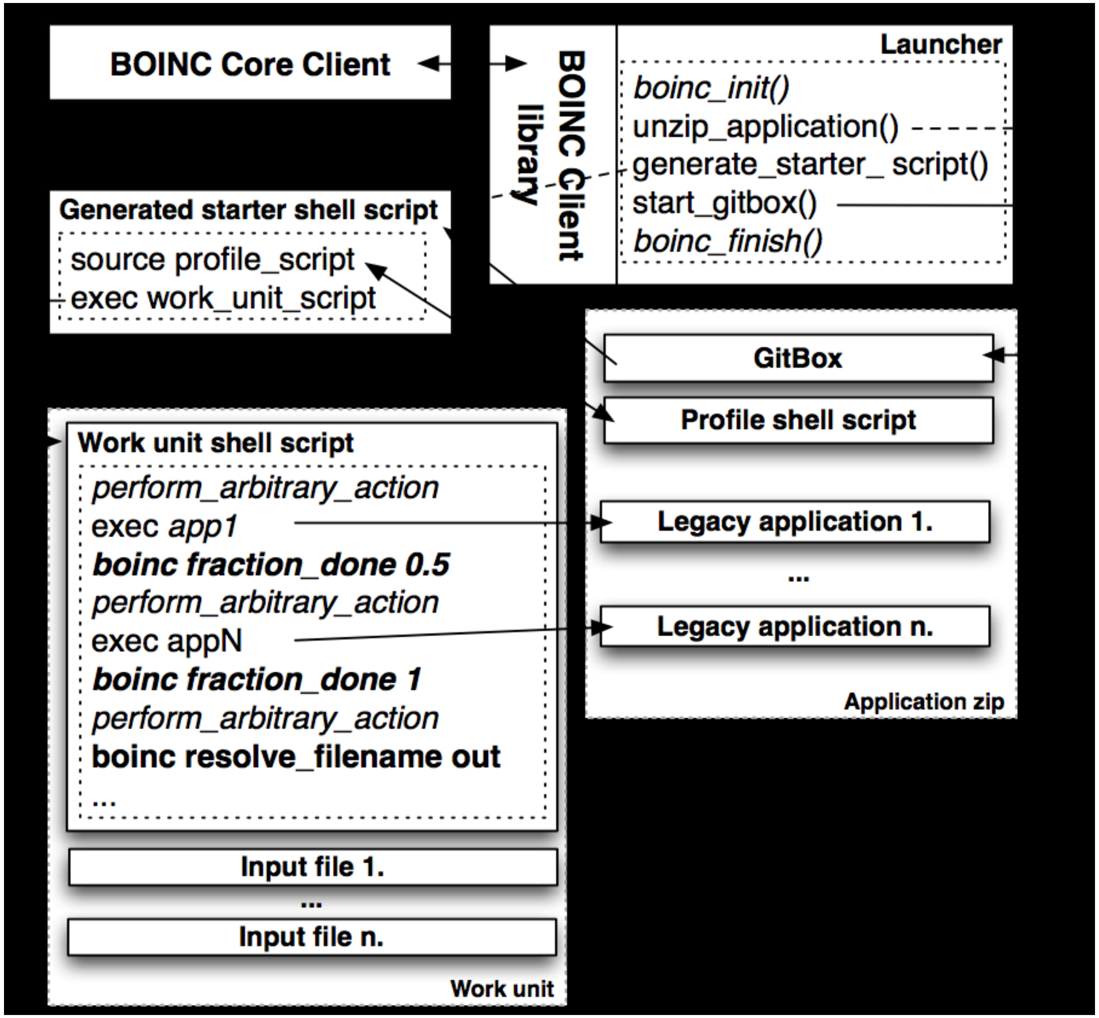
- DG successfully built with simulation consultant and deployed at client site

# SZDG/Simul8



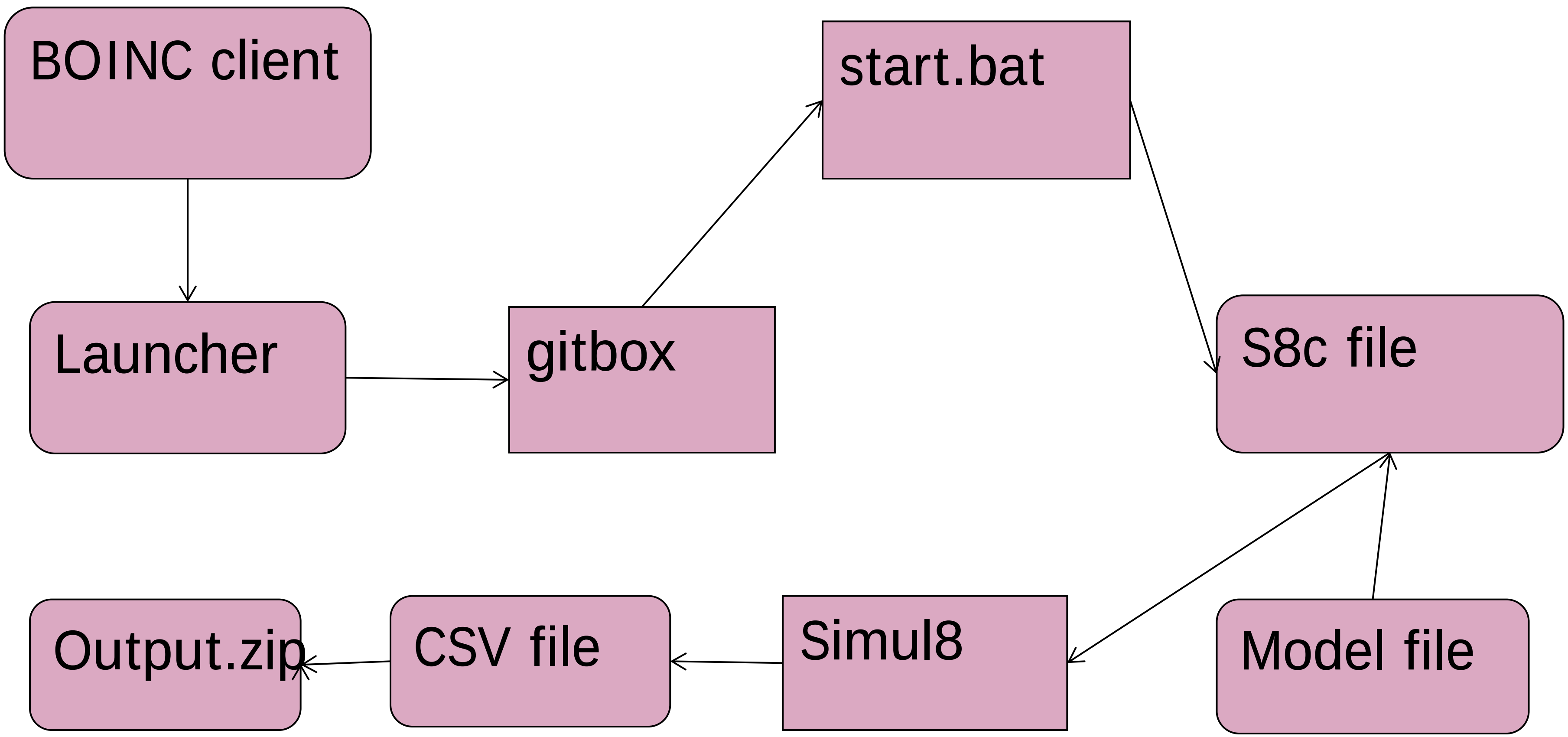
SZDG Server
WS-PGRADE (User Interface/ Portal)
Workflow
gUse (Workflow Processor & Services)
gUse DG Submitter
BOINC Server Components
Sched-uler
Data Server
BOINC Task DB
3G Bridge
Work Units
Tasks
BOINC Client
GenWrapper
Legacy Application
BOINC Client
GenWrapper
Legacy Application
BOINC Client
GenWrapper
Legacy Application
Workflow Desciption

# GenWrapper



BOINC Core Client
BOINC Client library
Launcher
boinc_init()
unzip_application()
generate_starter_ script()
start_gitbox()
boinc_finish()
Generated starter shell script
source profile_script
exec work_unit_script
GitBox
Profile shell script
Legacy application 1.
...
Legacy application n.
Application zip
Work unit shell script
perform_arbitrary_action
exec app1
boinc fraction_done 0.5
perform_arbitrary_action
exec appN
boinc fraction_done 1
perform_arbitrary_action
boinc resolve_filename out
...
Input file 1.
...
Input file n.
Work unit

# GenWrapper (simul8)



# Results

- Simul8 version
  - Emergency Room simulation (thanks Dr Vince Knight (Cardiff)!)
  - Each run 50 seconds
  - 3 runs per job
- Simul8 & Excel version (English!)
  - National Blood Service model
  - Each run 25 seconds
  - 4 runs per job
- In both cases speedup over 8 machines was around 5
- On-going analysis

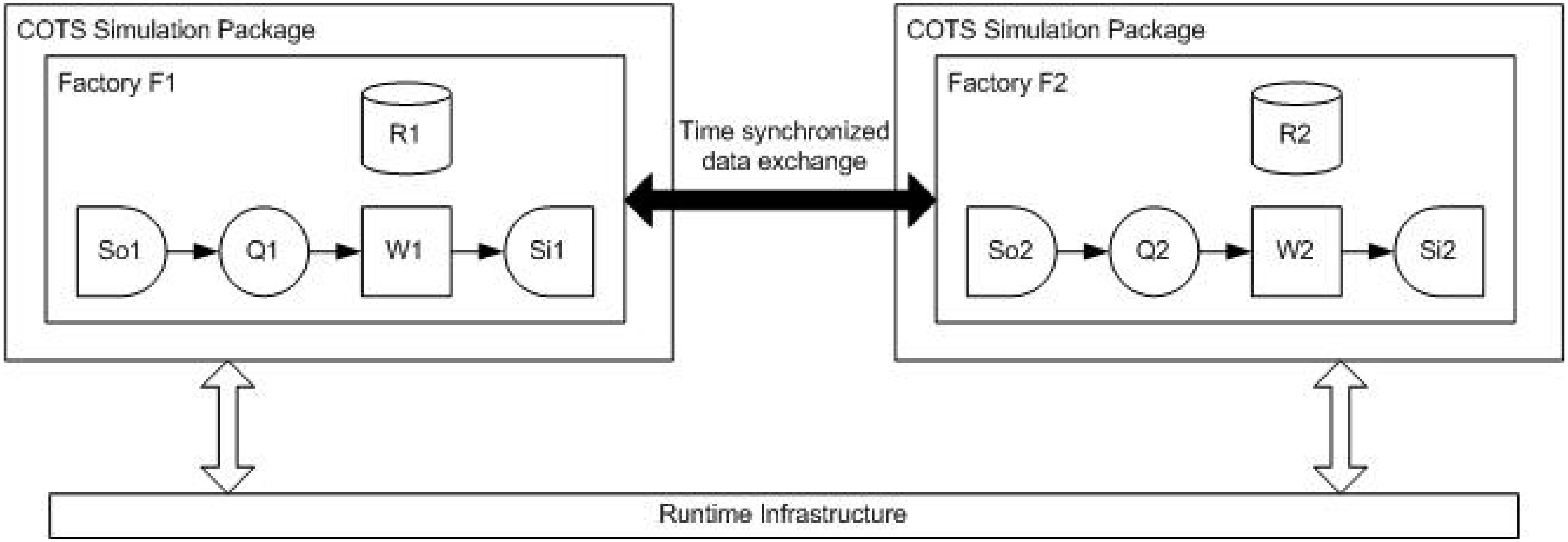
# e-Infrastructures for M&S
# High Speed Experimentation

- COTS Simulation Packages (and their ancillary software) can be supported
  - Small runtimes supported
  - License issues
  - Partnership with Vendor vital
  - SZDG Grid probably the best deployment architecture in a “standard” environment (simple to deploy and maintain)
  - Still need to integrate with an Experimentation Manager of some kind

# e-Infrastructures for M&S

## Simulation Interoperability/Distributed Simulation

Interoperability between (two +) CSPs during a simulation run



# e-Infrastructures for M&S

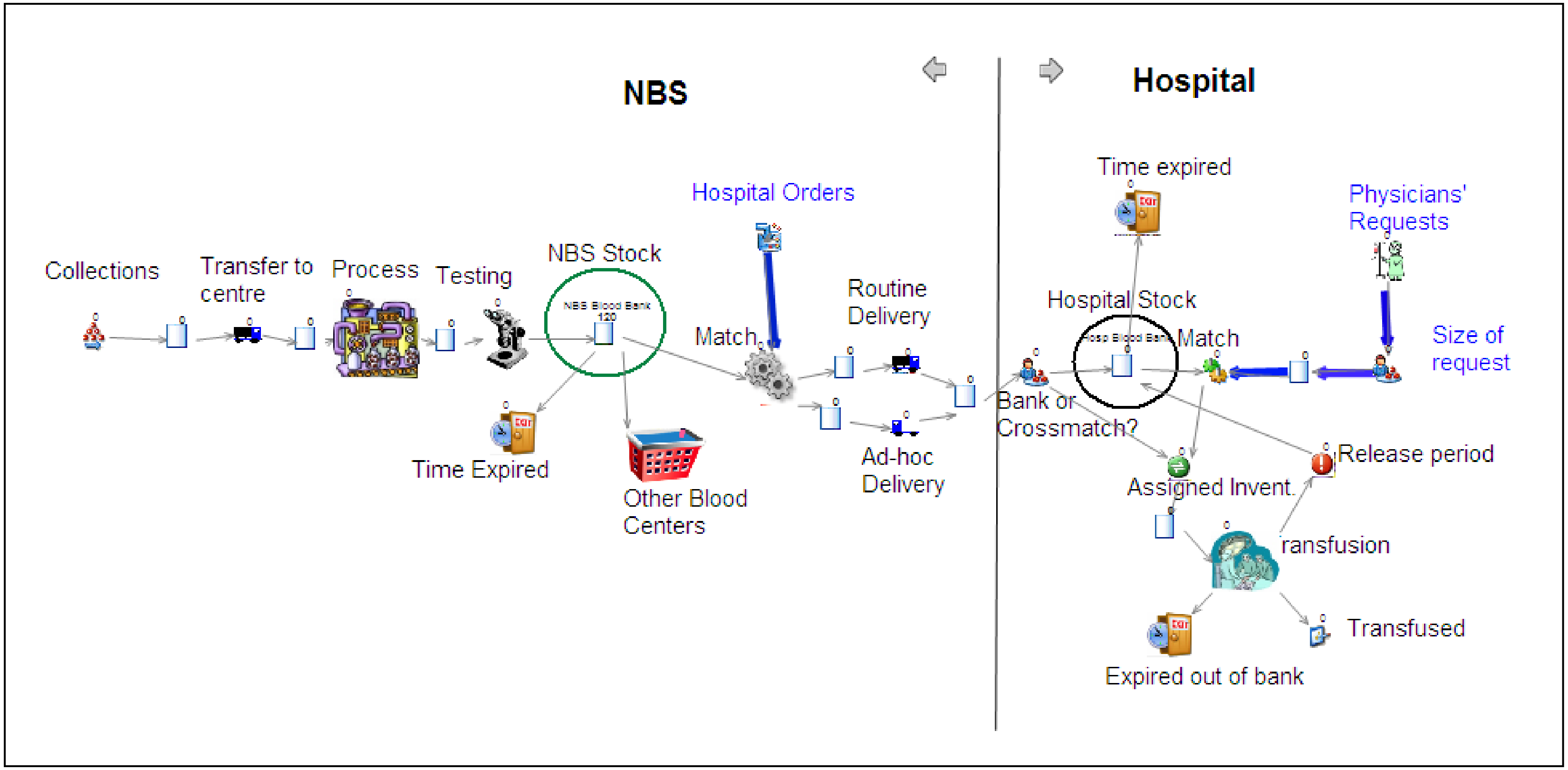
## Simulation Interoperability/Distributed Simulation

**Surveys**
Ryde and Taylor (2007) *WSC 2007*
Strassburger, et al. (2009) *WSC 2009*
Boer, et al. (2010) *Journal of Simulation*

- Motivations
  - Privacy
  - Data transfer/access problems
  - Model composability/update problems
  - Execution Time
- Illustrative case
  - Distributed simulation of blood supply chain
  - Korina Katsaliaki (UoT), Navonil Mustafee (Brunel), Sally Brailsford (Southampton), Mark Elder (Simul8)

Katsaliaki, et al. (2009) *JORS*, Mustafee, et al. (2009) *SIMULATION*
Taylor, et al. (2013) *ACM TOMACS*

# Simplified National Blood Service Model

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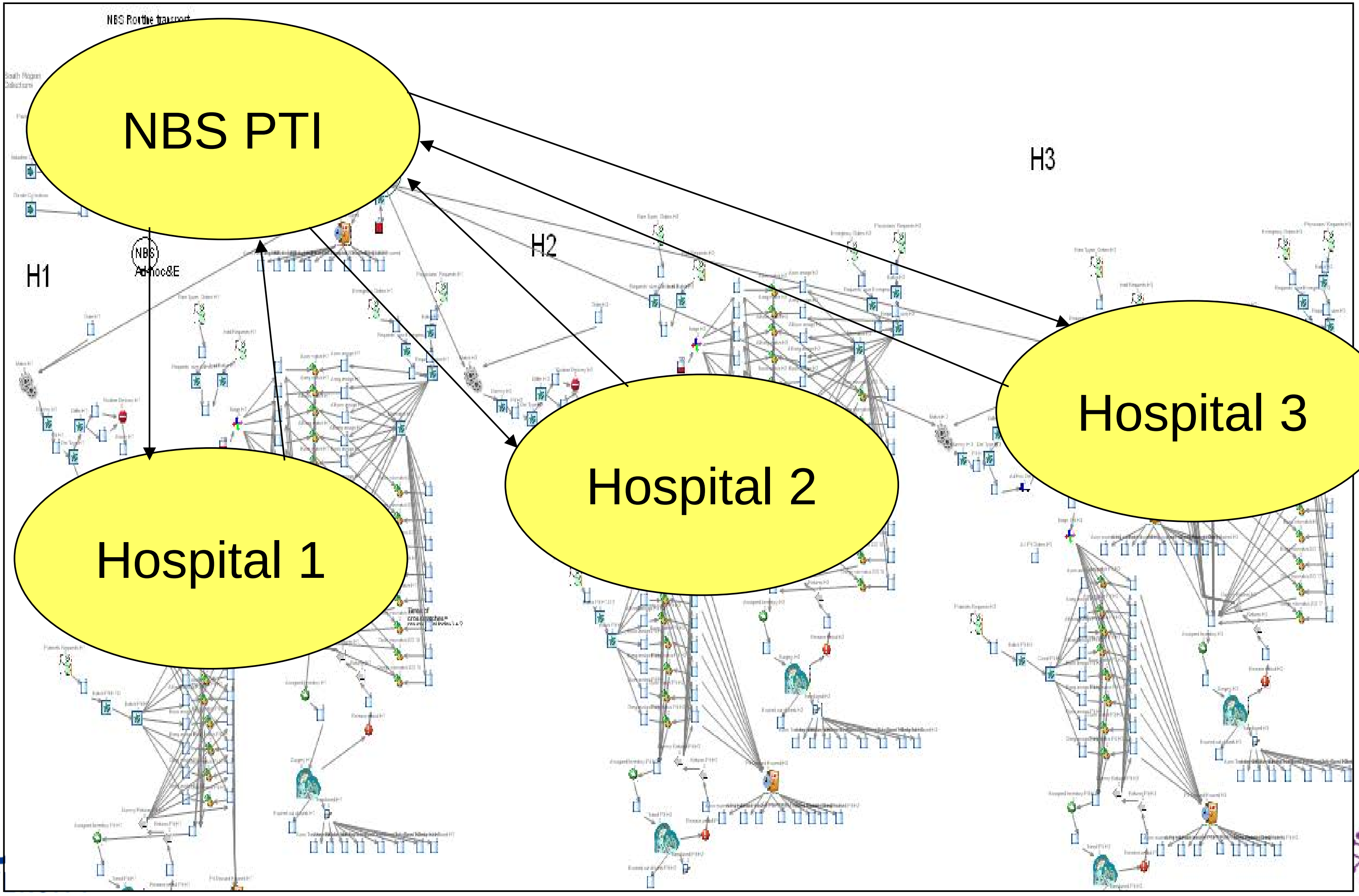
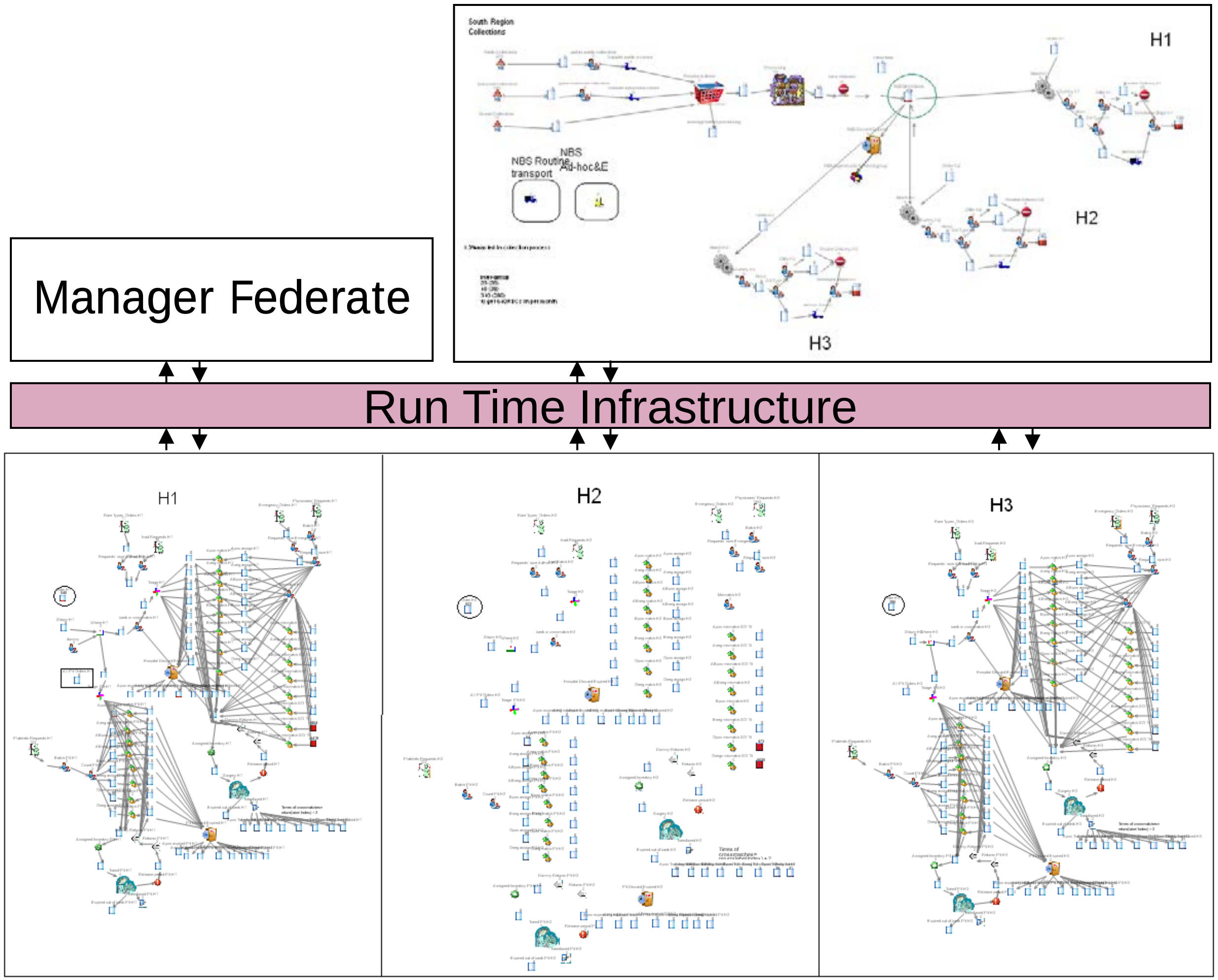
# Supply Chain of Blood



# Distributed Model



# CSP Controller Architecture – CSP Interfaces

- The CSP Controller Middleware utilizes the COM interface to access the Simul8 simulation engine

- COM interfaces used

  *MySimul8 As SIMUL8.S8Simulation*

  *MySimul8.Open*

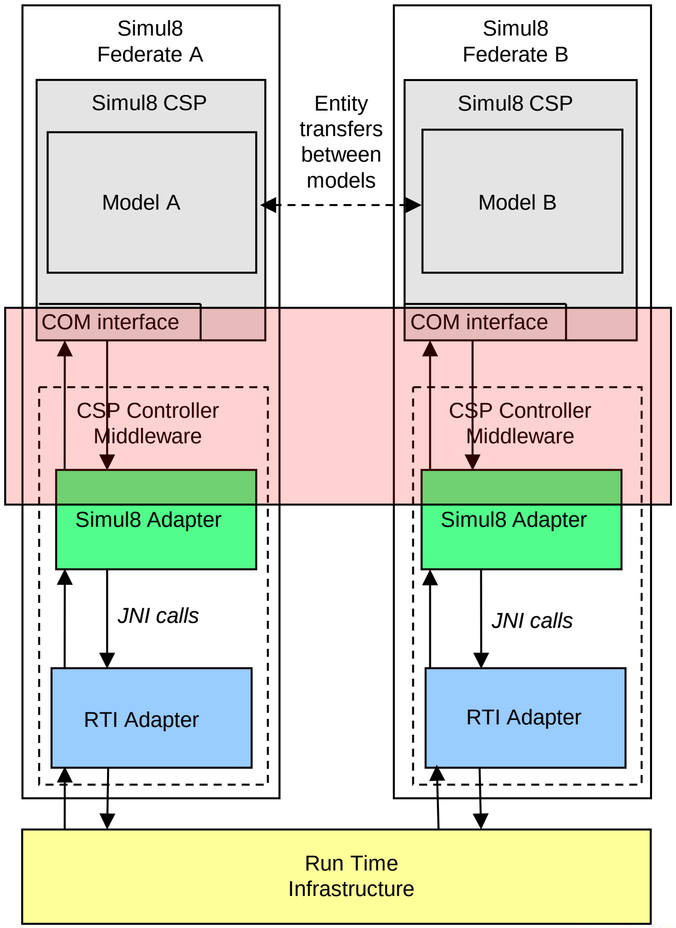
  *MySimul8.RunSim*

  *MySimul8.SimulationTime*

  *MySimul8.ExecVL*

  *MySimul8.StopSim*

  *MySimul8.Quit*

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# CSP Controller Architecture – HLA Interfaces

The HLA interface specification organises the communication between federates and the RTI into six different service groups

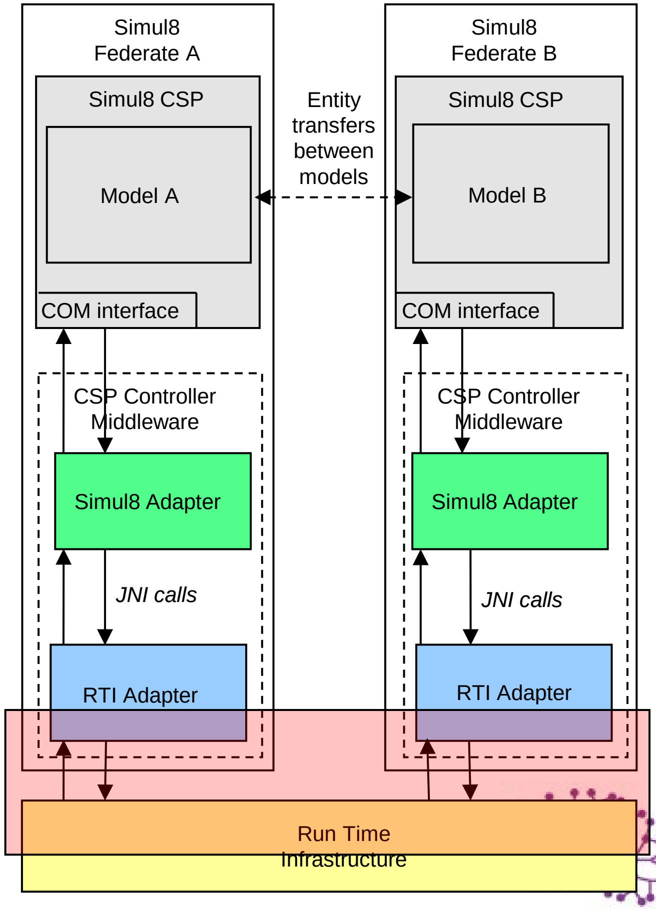
For our Type I IRM solution with Simul8 and the RTI we require HLA-defined services defined under the groups:

- Federation Management: RTI Calls for creation and deletion of federation; joining and resigning of federates from the federation; and creation and realization of synchronization points

- Declaration Management: Calls pertaining to publication and subscription of interactions

- Object Management: Calls that relate to sending and receiving interactions

- Time Management: RTI calls required to enable time constraint and time regulation and also to advance the federate simulation clock.

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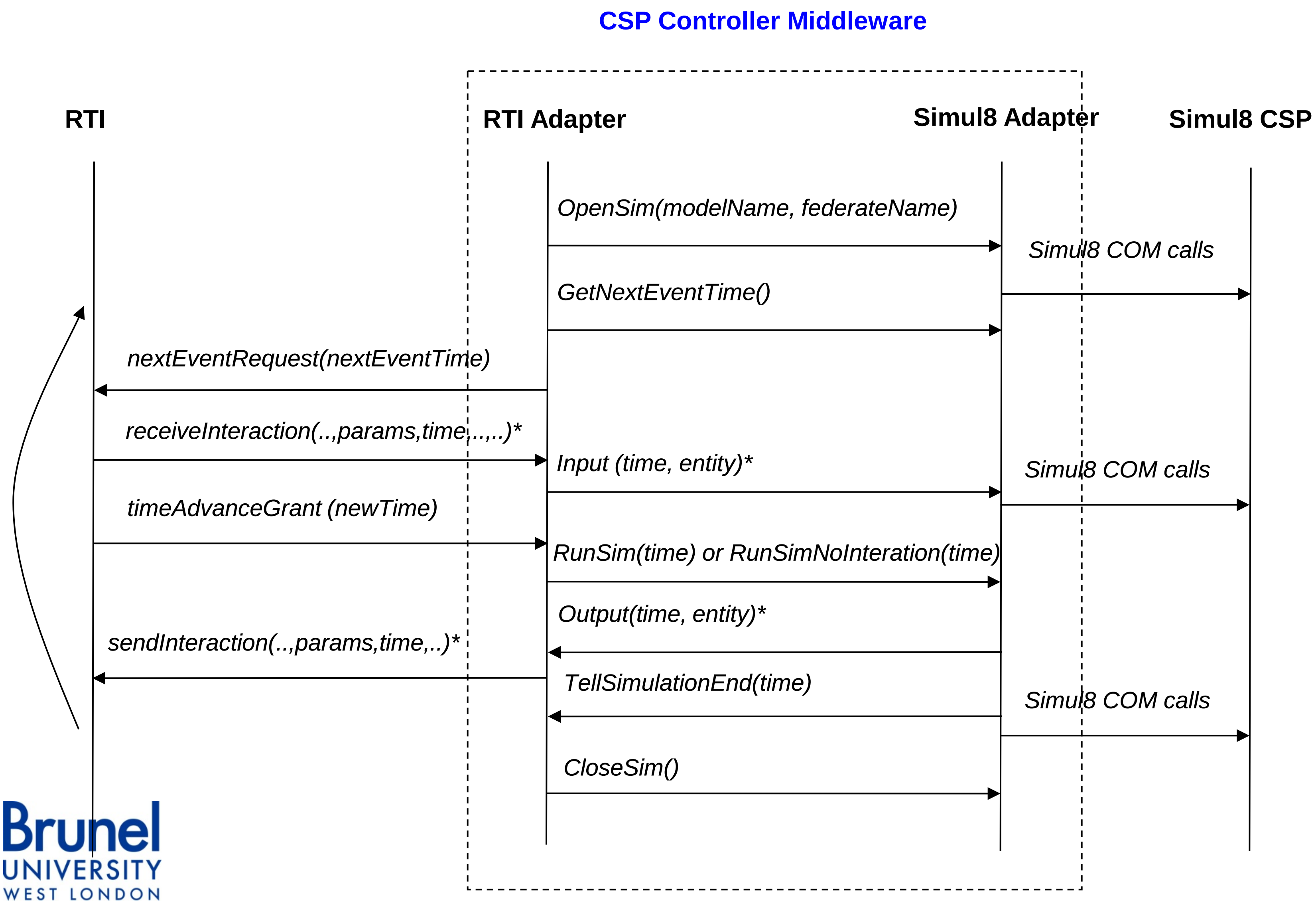
# CSP Controller Middleware Protocol

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# A Standards-based Approach

- COTS Simulation Package Interoperability Product Development Group under the Simulation Interoperability Standards Organization (SISO CSPI PDG)
- Roots in UK EPSRC GROUPSIM Project (2000-2004)
- Formal activity began June 2002
  - (HLA-)CSPIF (August 2002)
    - 16 international meetings, 80+ members
  - SISO Virtual Study Group (Jan 2003)
  - Final report submitted to SISO (Sept 2003)
  - Product Nomination submitted (June 2004)
  - PDG status awarded Oct 2004
  - Now transitioning to SISO CSPI PSG (www.sisostds.org)

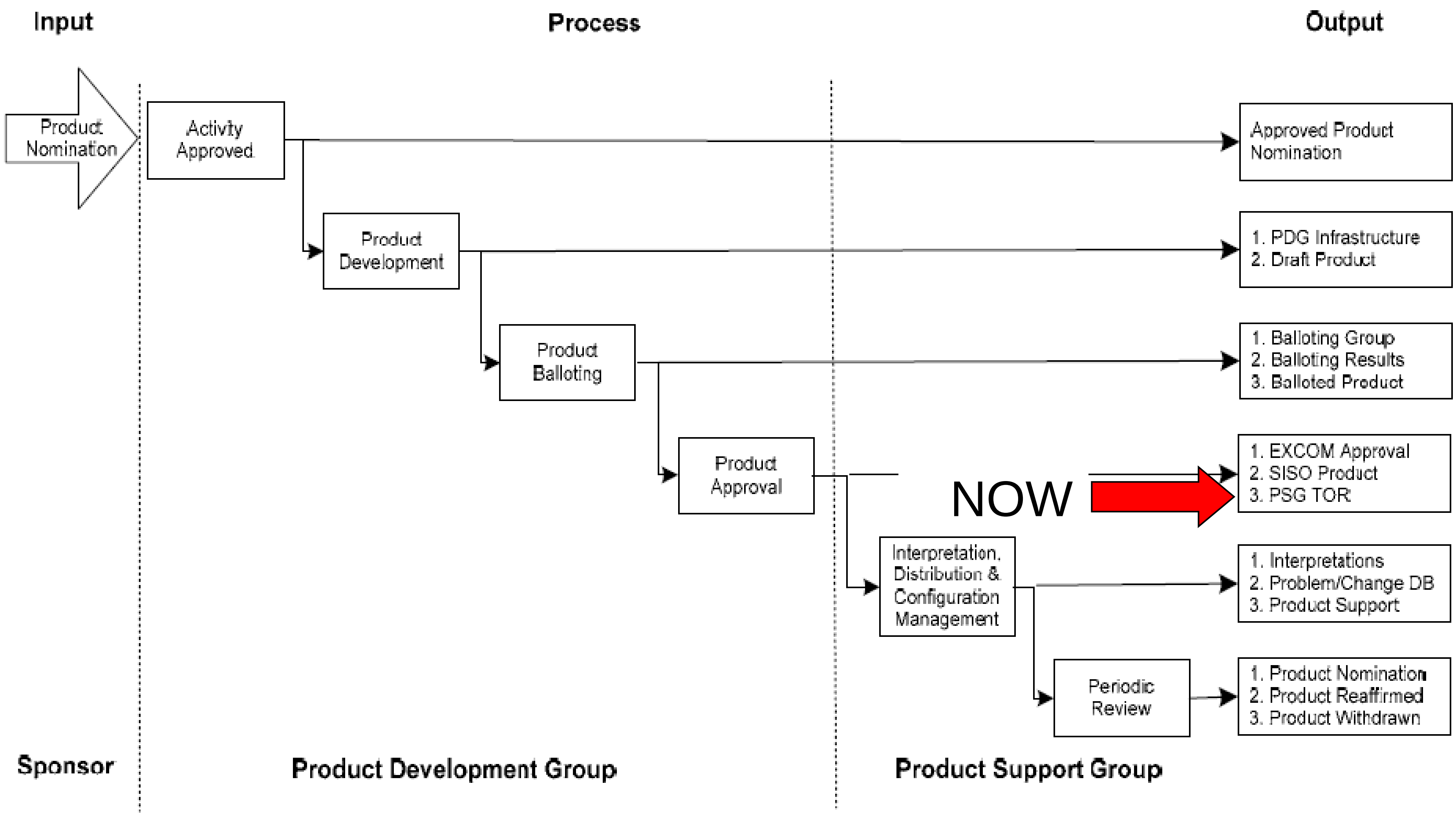



**Figure 1 - SISO Balloted Product Development and Support Process (BPDSP)**

# SISO CSPI PDG

- Aim
  - to develop standardised approaches to COTS Simulation Package Interoperability
- First major outcome
  - **Standard for COTS Simulation Package Interoperability Reference Models (SISO-STD-006-2010) (*Model-level interoperability*)**

**2008+ Literature**

**2008**
Taylor, et al. (2008a) *WSC 2008*, Taylor, et al. (2008b) *WSC* 2008, Mustafee and Taylor (2008a) *SW '08*, Mustafee and Taylor (2008b) *SW '08*
**2009**
Katsaliaki, et al. (2009) *Journal of the Operational Research Society*, Mustafee, et al. (2009) *SIMULATION*, Mustafee, et al. (2009) *Handbook of Research on Advances in Health Informatics and Electronic Healthcare Applications,* Taylor, S.J.E., et al. (2009) *WSC 2009*
**2010**
Taylor, S.J.E. et al. (2010) *WSC 2010*, Mustafee and Taylor (2010) *SW '10*, Taylor and Mustafee (2010) *Wiley Encyclopedia of Operations Research and Management Science*
**2011**
Taylor, et al. (2011) *WSC 2011*
**2013**
Taylor, et al. (2013) *ACM TOMACS*

# Interoperability Reference Models

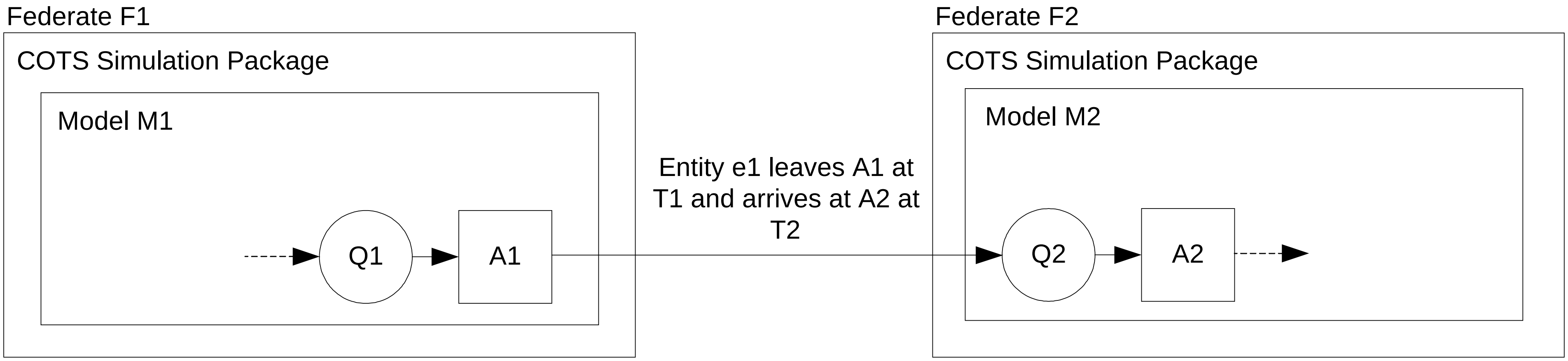
- Current list
  - Type A: Entity Transfer (3 IRMs)
  - Type B: Shared Resource
  - Type C: Shared Event
  - Type D: Shared Data Structure
- Previously appeared as
  - Type I: Asynchronous Entity Passing
  - Type II: Synchronous Entity Passing (Bounded Buffer)
  - Type III: Shared Resources
  - Type IV: Shared Events
  - Type V: Shared Data Structures
  - Type VI: Shared Conveyor

Standard for COTS Simulation Package Interoperability Reference Models (SISO-STD-006-2010)

# Interoperability Reference Models

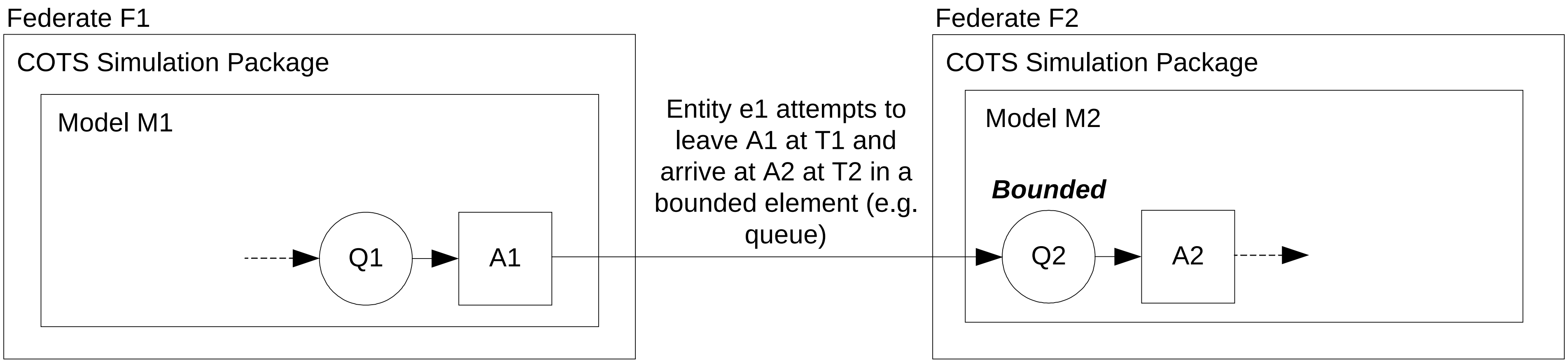
- Definition:
  - An interoperability problem *type* is meant to capture a general class of interoperability problem, while an *IRM* is meant to capture a specific problem within that class at the model level
- The purpose of an IRM is therefore:
  - to clearly *identify* the model/CSP interoperability *capabilities* of an *existing* distributed simulation
    - e.g. The distributed supply chain simulation is compliant with IRMs Type A.1, A.2 and B.1
  - to clearly *specify* the model/CSP interoperability *requirements* of a *proposed* distributed simulation
    - e.g. The distributed hospital simulation must be compliant with IRMs Type A.1 and C.1

# IRM Type A.1 General Entity Transfer



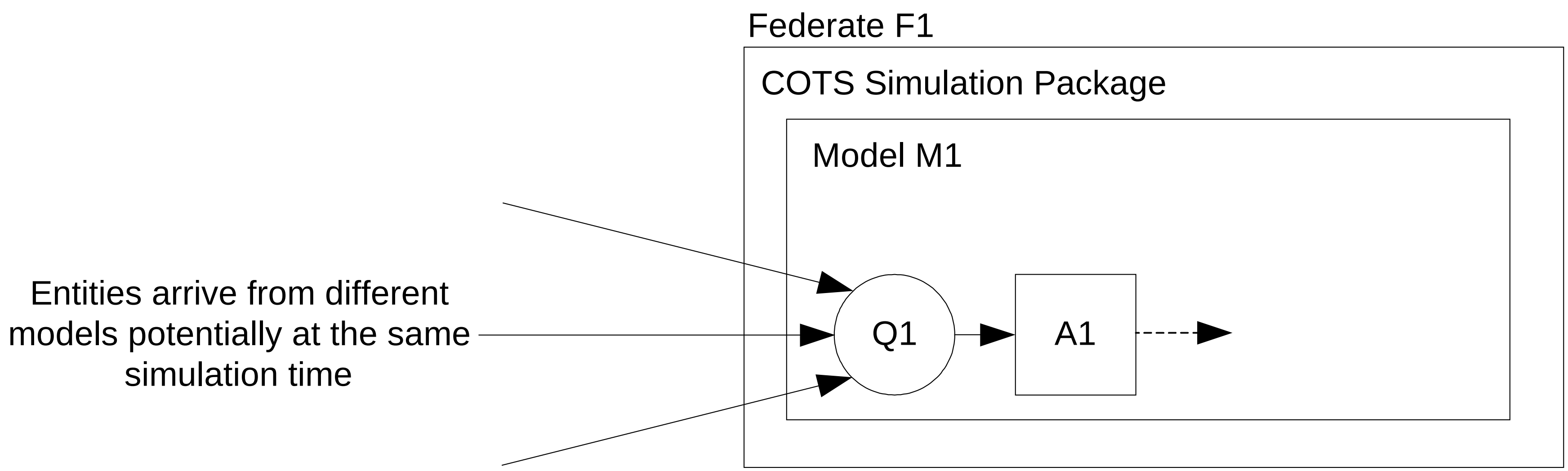

T1 =< T2 or T1<T2?

# IRM Type A.2 Bounded Receiving Element




Must account for blocking behaviour

# IRM Type A.3 Multiple Input Prioritization




The priority rules must be specified and be strictly observed

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# Blood supply chain…

- Orders/Blood units are only exchanged
- In terms of interoperability…
  - Distributed NBS model has the functionality of
    - IRM A.1, T1>=T2 (Entity Transfer)
  - Currently does not have the functionality of
    - IRM A.3 (Ordered Queues)
  - Does not require the functionality of
    - IRM A.2 (Bounded buffer)
- Specification then produced in IRL and a FOM and agreed by all parties before implementation

**Some other examples**

Gan, et al. (2005) *WSC 2005,* Taylor, et al. (2007) *WSC 2007,* Rabe, et al. (2006) *WSC 2006,* Lenderman, et al. (2007) *Journal of Simulation,* Strassburger, et al. (2007) *WSC 2007,* Raab, et al. (2007) *WSC 2007,* Jain, et al. (2009) *WSC 2009,* Son, et al. (2009) *Journal of Simulation* Pedrielli, et al. (2011) *PADS 2011*

# e-Infrastructures for M&S

## Simulation Interoperability/Distributed Simulation

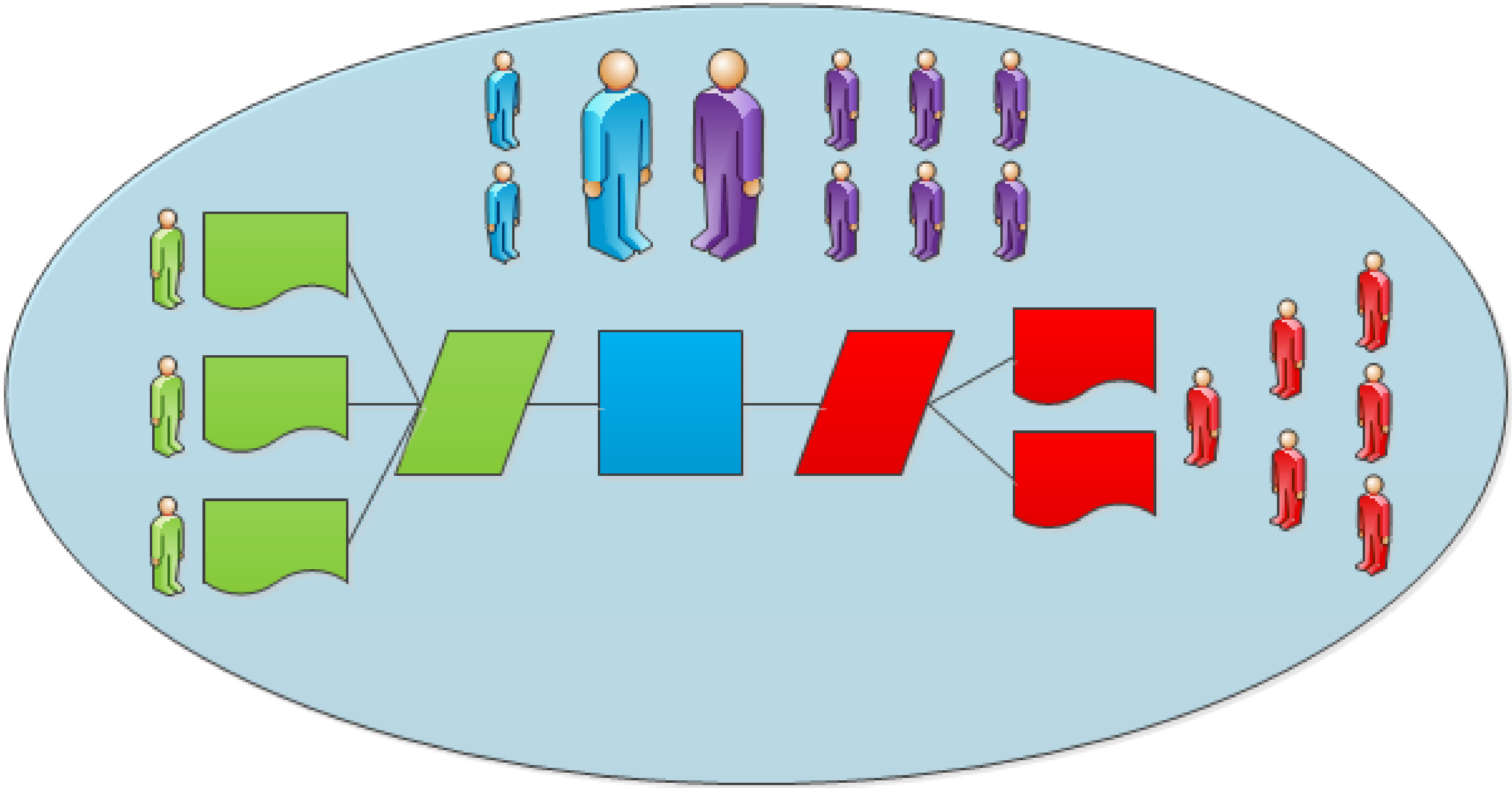
- Entirely possible but needs
  - Better COTS Simulation Package Integration
  - More standardisation
  - HLA RTI software cost?

# e-Infrastructures for M&S

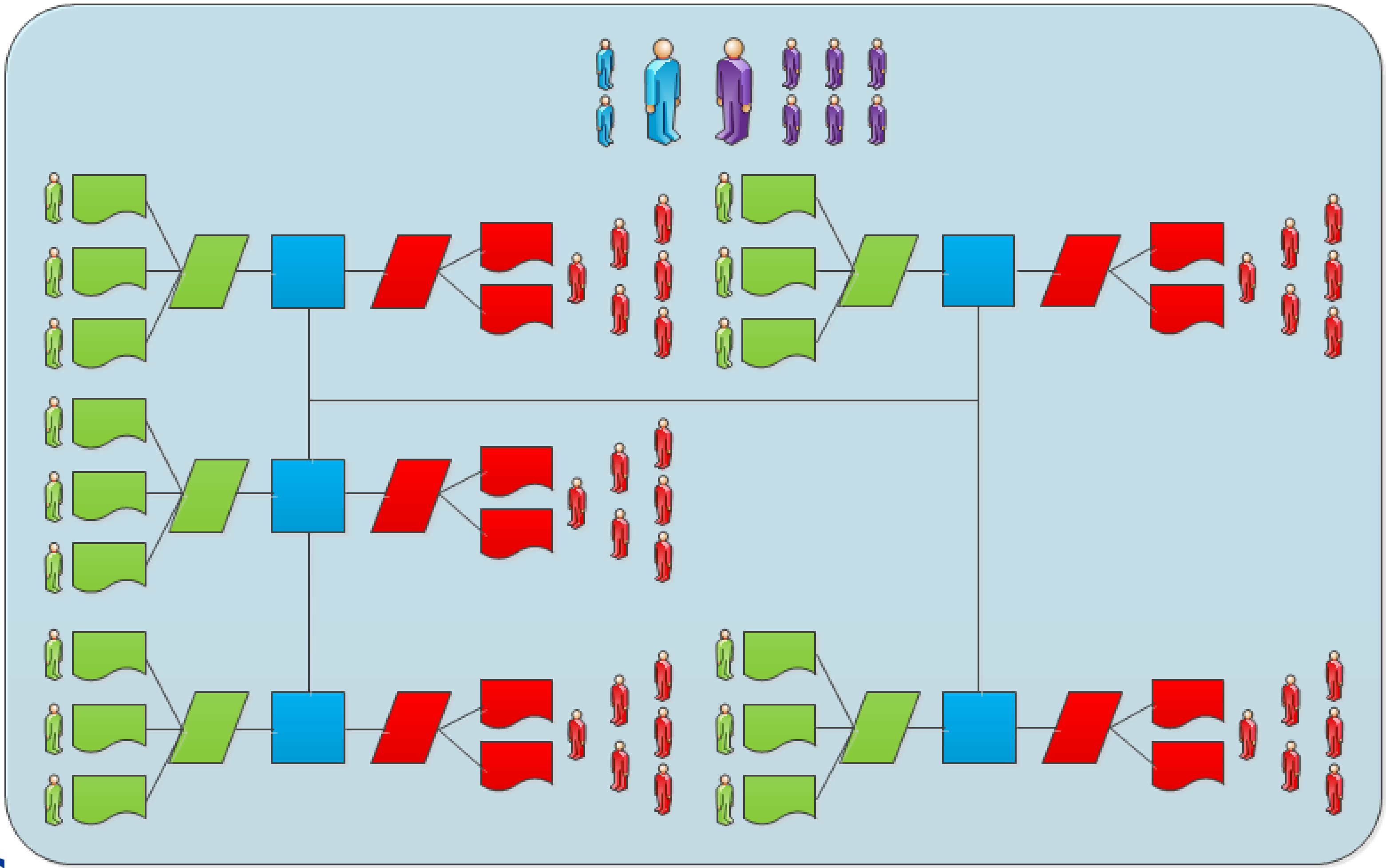
## Data (Artefact) Management

- Project cost reduction by better management of all simulation project artefacts
- Integration with other projects
- Cheaper model development through reuse

# A "typical" M&S project



# However, models are getting larger…



# In reality, in a large system…

- E.g. Healthcare
  - One or more emergency room models
  - One or more outpatient models (othopaedics, urology, etc.)
  - Ambulance models
  - Social care models
  - Pathway models
  - Health economics models/studies
- Overlap in terms of data, model elements, model scope, results and people

# Initial attempt

- DEMO ontology (Fishwick and Miller)
  - Discrete event ontology
- DESC
  - Discrete event simulation component ontology
  - Basic search and discovery architecture


Taylor, S.J.E., et al. (2010). *Organizational Advancements through Enterprise Information Systems: Emerging Applications and Developments.* 336-352.
Bell, D., et al. (2008). *International Journal of Enterprise Information Systems*. 4 (4), 47-61.

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# e-Infrastructures for M&S

## Data (Artefact) Management

- Experience shows that ontology development is very difficult
  - Automatic extraction
- No solution as the problem needs to be properly conceptualised
  - Arguably a methodology is required prior to the technology
  - Namespace conventions
  - Is a centralised organisational “authority” possible given multiple modellers?

# Conclusions
# e-Infrastructures for M&S

- An *e-Infrastructure for M&S* (in the context of this talk) is
  - an environment where resources — COTS simulation packages and ancillary software (e.g. Excel), models, data etc. — are readily accessible and can be easily shared and/or interoperated
  - It integrates networks, grids, middleware, computational resources, data repositories, and software tools within (virtual) organizational boundaries
- In this domain of simulation
  - Is it worth it?  Is it possible? How long?

# Conclusions
# e-Infrastructures for M&S

- Collaborative Support
  - Benefit: **High**
  - Possible: **Easy!**
  - Time: **Now**
- High Speed Experimentation
  - Benefit: **High**
  - Possible: **Yes**, with some investment
  - Time: **Near term**

# Conclusions
# e-Infrastructures for M&S

- Simulation Interoperability/Distributed Simulation
  - Benefit: Evidence suggests in some cases **high**
  - Possible: **Yes**, with more research/ standardisation
  - Time: **Medium term**
- Data (Artefact) Management
  - Benefit: **High**
  - Possible: **Very challenging**
  - Time: **Long term**

# Conclusions
# e-Infrastructures for M&S

- Real benefit
- Would consist of
  - Groupware
  - Grid/cloud desktop grid(s)
  - Support for simulation interoperability/distributed simulation
  - Artefact management
- Integration?
  - Grid supporting simulation interoperability… not normally found in e-Infrastructures
- Real world problems are key to understanding actual requirements
- End user/Vendor participation is absolutely required

# (Main) Acknowledgements


- **Systems Biology**
  - Xuan Liu, David Gilbert, Jun Wang, Quan Jao (Brunel), Navonil Mustafee (Swansea)
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- **NBS Case Study**
  - Korina Katiaslaki (UoT), Navonil Mustafee (Swansea), Sally Brailsford (Southampton), Mark Elder (Simul8)
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  - Steffen Strassburger (IUT), Stephen Turner (NTU), Navonil Mustafee (Swansea), Malcolm Low (D-SIMLAB), John Ladbrook (Ford), Markus Rabe (IPK), Tomas Schulze (Magdeburg), Wentong Cai (NTU), Frank Riddick (NIST), Katherine Morse (SISO), Rick Servinghaus (SISO), Rockwell, Simul8, Lanner, CSPI PDG and SISO people (esp. 3 TADs!)


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