The NERC Cluster Grid

Dan Bretherton, Jon Blower and Keith Haines

Reading e-Science Centre
www.resc.reading.ac.uk
Environmental Systems Science Centre
University of Reading, UK

NATURAL ENVIRONMENT RESEARCH COUNCIL
ENVIRONMENTAL SYSTEMS SCIENCE CENTRE

The University of Reading

e-ReseaRCH SOUTH

Reading e-Science Centre

Outline of presentation

- What is a grid?
- Running climate models on HPC clusters belonging to other institutes
  - Climate models: Challenges for grid middleware
- G-Rex grid middleware
  - The climate scientist's view
  - The grid administrator's view
- The NERC Cluster Grid

e-Research SOUTH

STFC + Reading, Southampton and Oxford universities

Some grid related organisations

- NERC e-Science Centres
  - Reading e-Science Centre (ReSC) - http://www.resc.reading.ac.uk/
  - National Institute for Environmental e-Science (NIEeS) - http://www.niees.ac.uk/
    - GridInfo: http://www.niees.ac.uk/grid_info.shtml
- e-Research South - http://www.eresearchsouth.ac.uk/
- National Grid Service (NGS) - http://www.grid-support.ac.uk/
- National e-Science Centre (NeSC) - http://www.nesc.ac.uk/

A definition of “grid”

- From the NIEeS web site:
  - [A grid] “allows sharing of computing, application, data and storage resources”.
  - “Grids…
    - cross geographic and institutional boundaries
    - lack central control
    - are dynamic
      - (computers join and leave in an unco-ordinated fashion).“

Wide scope of grid computing

- From Mike Mineter's presentation at NGS Application Developer's Course, NeSC Feb '07

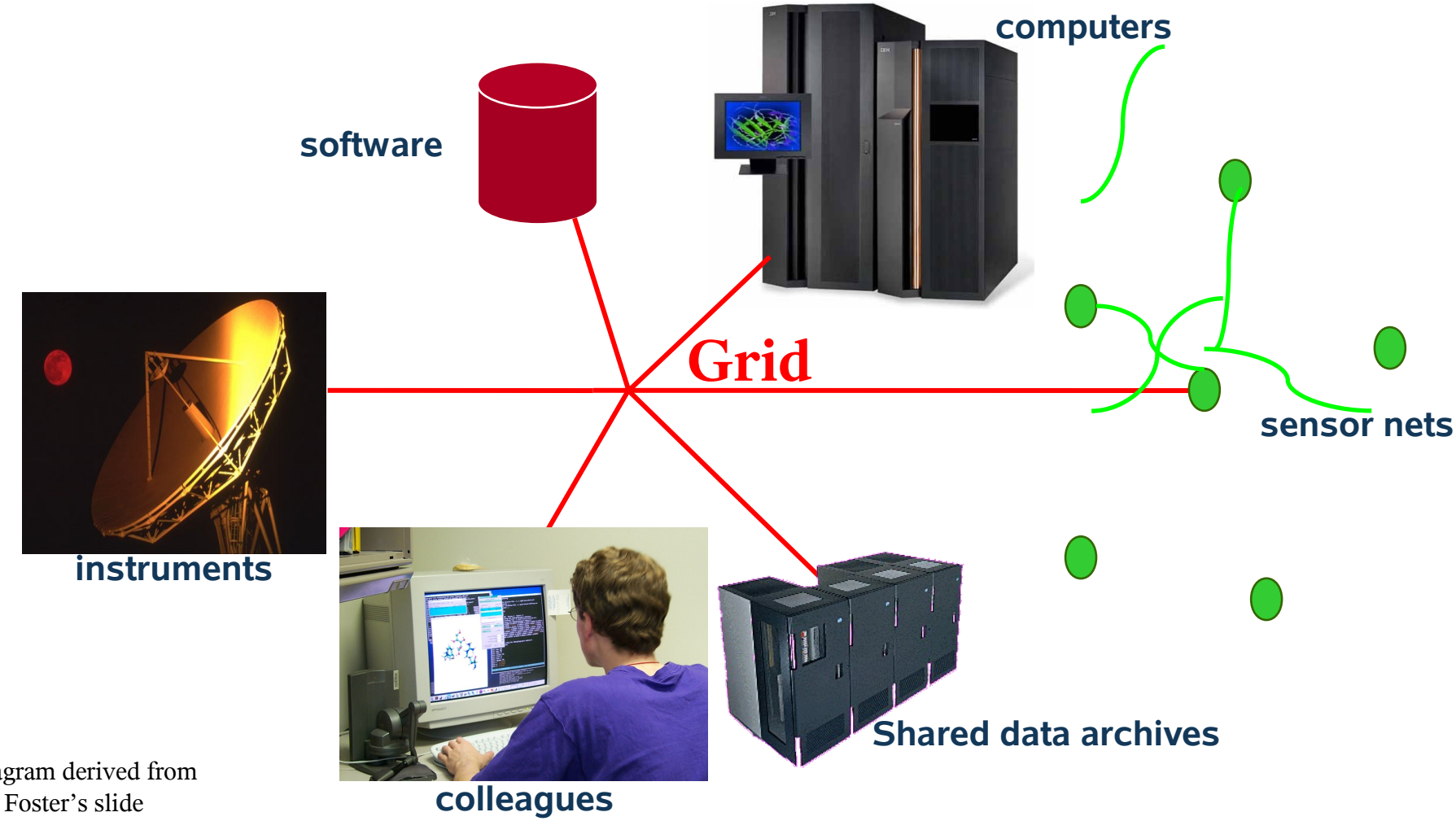


Diagram derived from
Ian Foster's slide

Wide scope of grid computing

- From Mike Mineter's presentation at NGS Application Developer's Course, NeSC Feb '07

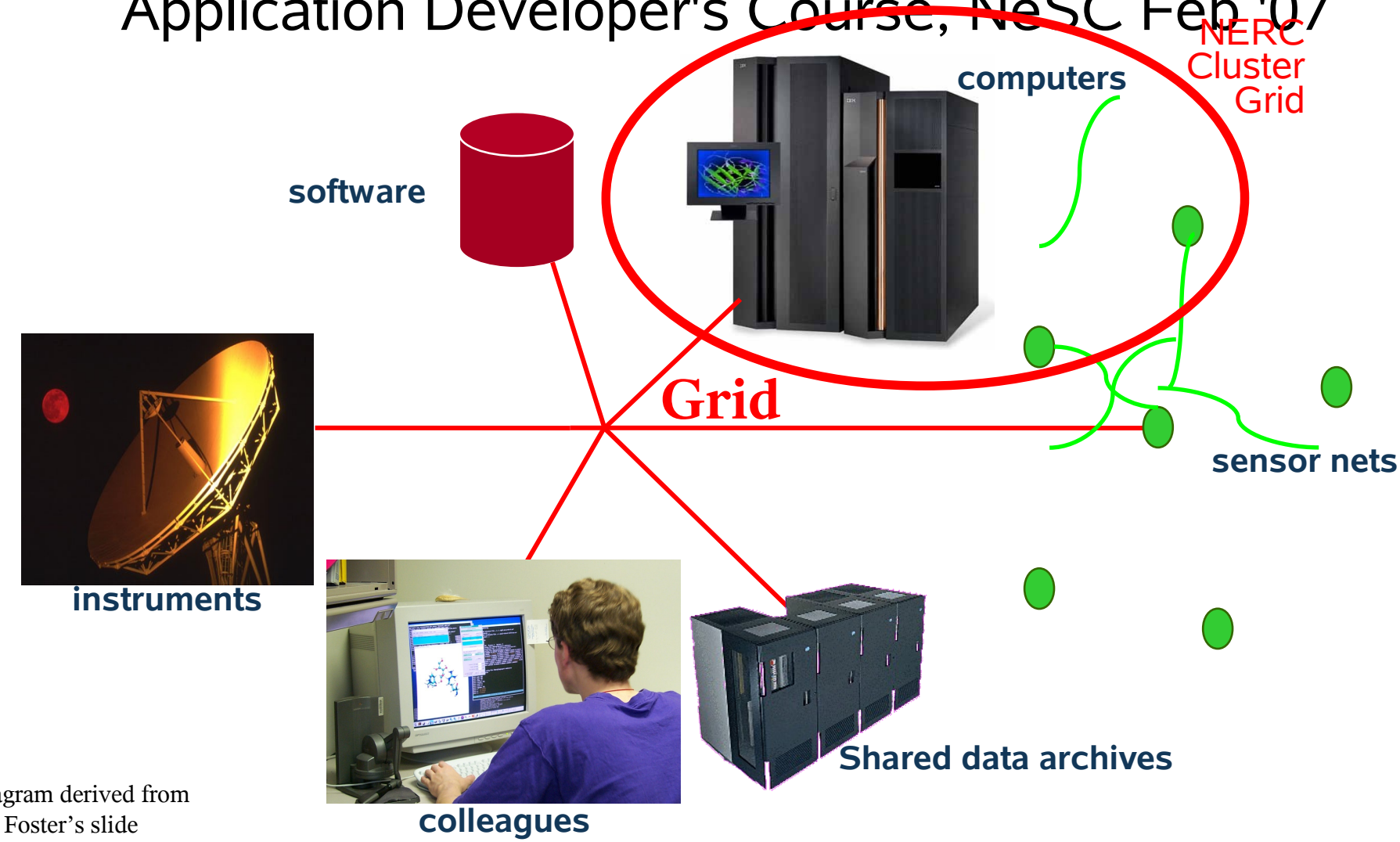


Diagram derived from
Ian Foster's slide

Computational challenges of climate models

- Typical requirements
  - Parallel processing (MPI) with large number of processors (usually 20-100)
  - Long runs lasting several hours, sometimes days
  - Large volumes of output
  - Large number of separate output files

NEMO Ocean Model

- Main parameters of a typical 1/4° Global Assimilation run for **one year**:
  - Run with 80 processors
  - 48 hours per model year on a typical cluster
- Outputs 4 GB in 1000 separate files as diagnostics every 40 minutes
- Output for a one year run is roughly 300 GB, a total of 75000 separate files
  - But, disk quota on remote cluster is only 250 GB
- 50-year `Reanalysis` = 15 Tb

NERC climate community's grid middleware requirements

- Background
  - Many NERC institutes have their own HPC clusters
  - Scientific collaborations benefit from sharing cluster resources
    - Scientists already doing this quite happily in traditional way
- The scientist's grid middleware requirements:
  - Deal with problem of small disk quotas on remote clusters
  - Minimal changes to scientific work-flow scripts
- The grid administrator's middleware requirements
  - Easy to set up and maintain
  - Minimal involvement of remote cluster administrators

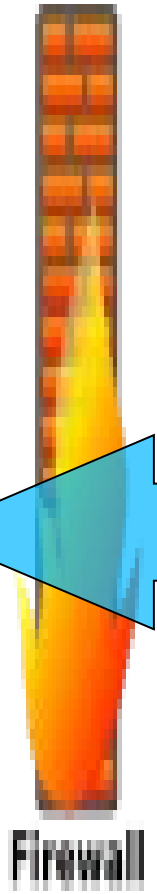
G-Rex (Grid Remote Execution)

- Successor to Styx Grid Services
- "Light weight" middleware implemented in Java
  - Platform independent (but only tested on Linux)
- G-Rex *server* is a Web application
  - Runs inside a servlet container (only tested Apache Tomcat)
  - Allows applications to be exposed as Web services
- G-Rex *client* is command line program `GRexRun`
  - Behaves as if remote model were actually running on user's own computer
    - Remote model's output becomes output from GRexRun
    - Waits until end of model run before exiting

Deployment of a NEMO G-Rex service

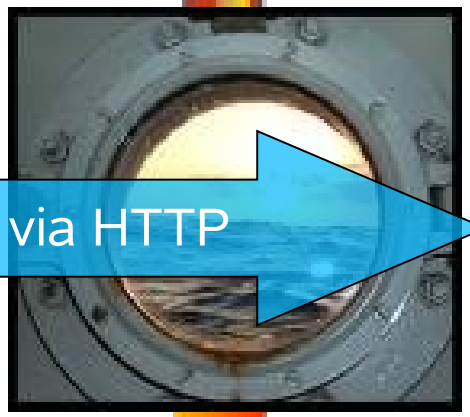
Client

Server



Input and output via HTTP

Tomcat
port open
to client



Apache
Tomcat

NEMO model setup, including source code, work-flow scripts, input data and output from all runs

NEMO
launch scripts and
forcing data
(same every run)

NATURAL ENVIRONMENT RESEARCH COUNCIL
ENVIRONMENTAL SYSTEMS SCIENCE CENTRE

The University of Reading

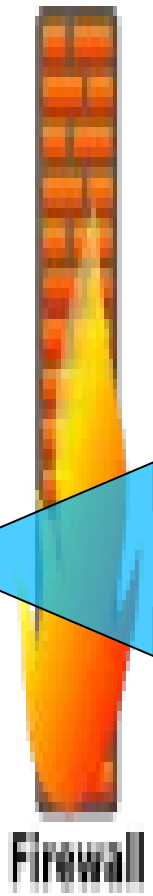
e-ReseaRCH SOUTH

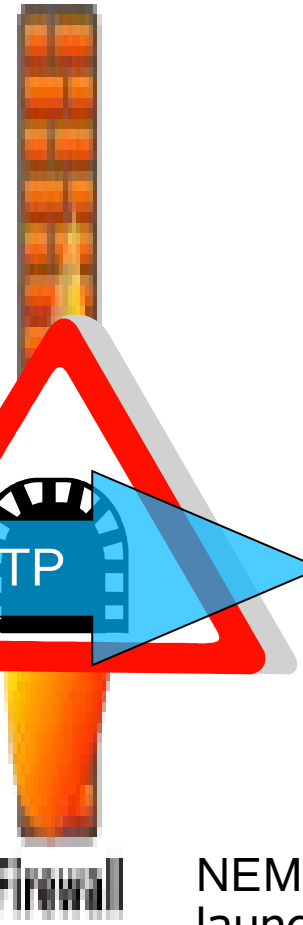
Reading e-Science Centre

NEMO service: SSH tunnel instead of open port

Client

Server

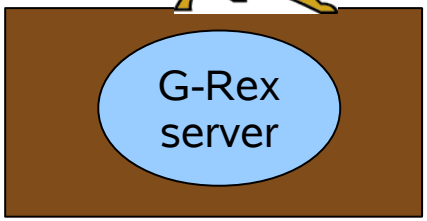




SSH
tunnel

Input and output via HTTP

Apache
Tomcat



NEMO
launch scripts and
forcing data
(same every run)

NEMO model setup, including source code, work-flow scripts, input data and output from all runs

NATURAL ENVIRONMENT RESEARCH COUNCIL
ENVIRONMENTAL SYSTEMS SCIENCE CENTRE

The University of Reading

e-RESEARCH SOUTH

Reading e-Science Centre

G-Rex features important to scientists

- Output transferred back to user during model runs
  - Job can be monitored easily
    - Defective jobs identified early – avoids wasting CPU time
  - No data transfer delay at end of run
- Files deleted from server when transfer completed
  - Minimises accumulation of model output data
- GrexRun easily incorporated into existing scripts
  - `GRexRun` usually replaces `mpirun`
  - A typical `GRexRun` command to run NEMO model:

```
grexrun.sh http://user:passwd@host:port/GRex/nemo
  input.tar.gz ORCA025
  --drm-walltime 7:00:00 --drm-procs 81
```

Important for grid administrator - easy server installation and setup procedure:

- Installation
  - Download tarball from Sourceforge and unpack

http://grex.svn.sourceforge.net/viewvc/grex/trunk/G-Rex

  - Download and unpack Sun Java and Apache Tomcat
  - Copy `G-Rex/code/dist/G-Rex.war` to Tomcat's `webapps`
  - Talk to cluster's firewall admin. (SSH tunnel or open port?)
- Setting up a service
  - Write model launch script containing `mpirun` command
  - Add a section in `GRexConfig.xml` for each service; specifies:

(1) model launch script (2) input & output file patterns

(3) expected and optional arguments (4) flagged options

NERC Cluster Grid

- 1600 processors in 5 clusters
  - (1) ESSC - 64 processors (2) BAS - 160 (3) PML - 344 (4) POL – 360 (5) NOC - 780
- G-Rex services
  - NEMO model: build and execution services
  - NEMO utilities: Data interpolation and aggregation
  - POLCOMS model: build and execution services
  - `qstat` (http://lovejoy.nerc-essc.ac.uk:8080/GridPortal/Portal)
  - `qdel`
  - Other services – requests & suggestions welcome
- Ganglia load and performance monitoring system
  - See Web frontend: http://www.resc.rdg.ac.uk/ganglia/

Acknowledgement & Summary

- **Thanks to NERC cluster admins. for interest and support of NERC Cluster Grid project**
- Climate models produce lots of data
  - Usually much more than quota on other institutes' clusters
- G-Rex grid middleware has 3 key features:
  - Transfers output during runs, deletes from server
  - `GRexRun` easily integrated into scientific work-flow scripts
  - Web services easy to install and maintain
- NERC Cluster Grid – 1600 procs, 5 clusters
  - G-Rex services for NEMO and POLCOMS

NATURAL ENVIRONMENT RESEARCH COUNCIL
ENVIRONMENTAL SYSTEMS SCIENCE CENTRE
The University of Reading
e-ReseaRCH SOUTH
Reading e-Science Centre