The NERC Cluster Grid

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Dan Bretherton, Jon Blower and Keith Haines

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

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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

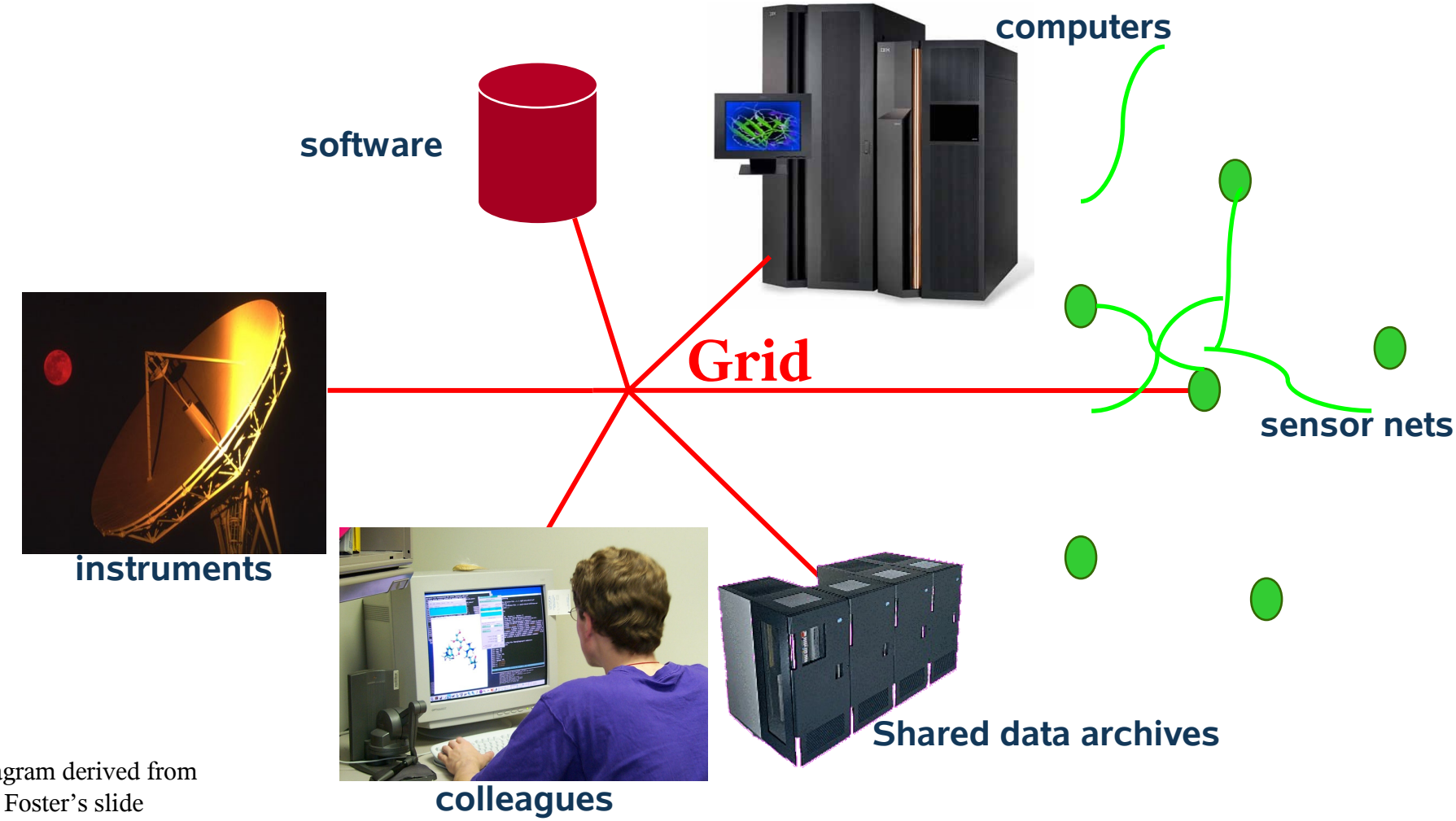

Diagram derived from
Ian Foster's slide

Wide scope of grid computing

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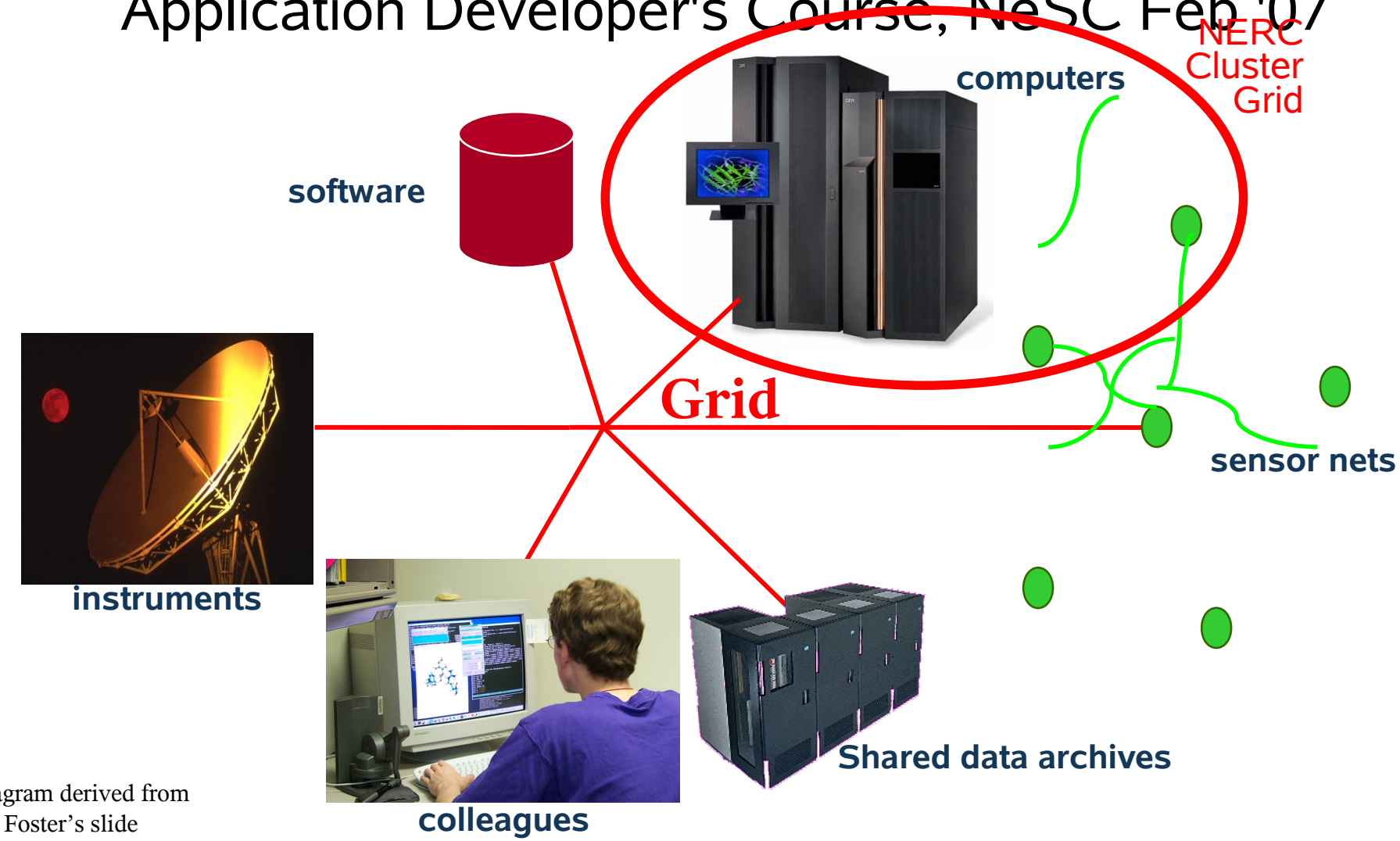

Diagram derived from
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Computational challenges of climate models

- 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

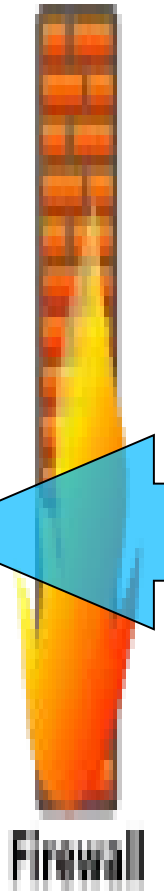
G-Rex (Grid Remote Execution)

- 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

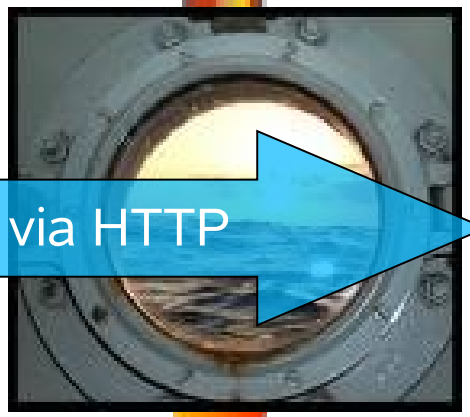
Deployment of a NEMO G-Rex service

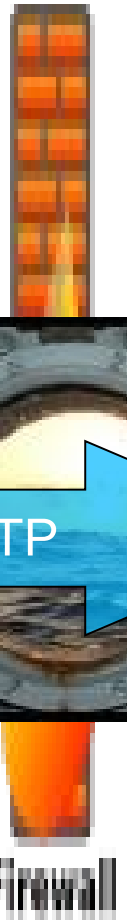
Client

Server



Tomcat
port open
to client





Apache
Tomcat

Input and output via HTTP

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)

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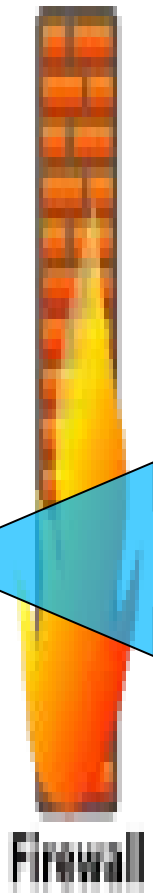
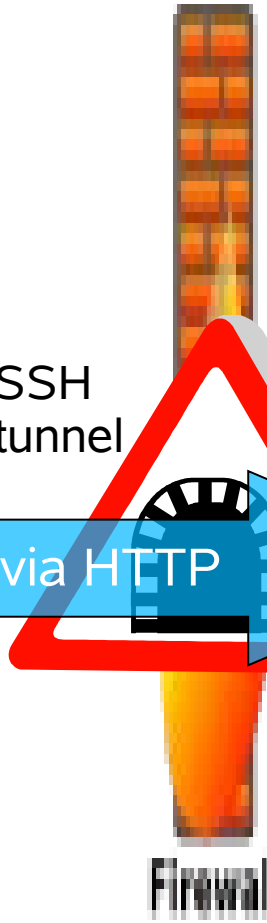
NEMO service: SSH tunnel instead of open port

Client

Server





SSH
tunnel

Input and output via HTTP

Apache
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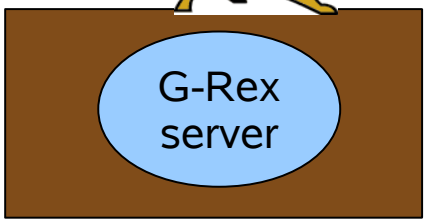

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G-Rex features important to scientists

- 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

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