



ARCHIE-WeSt

**ARCHIE-WeSt: A Big Computer for
Big Projects at Strathclyde and
the West of Scotland**

www.archie-west.ac.uk





Who we are



We are a supercomputer centre for the West of Scotland based at the University of Strathclyde dedicated to wealth creation and research excellence in the region. Funded by EPSRC, we operate in partnership with the **Universities of Glasgow, Glasgow Caledonian, West of Scotland and Stirling.**

The aim of the centre is to **support multi-disciplinary research**, with a centre of gravity in engineering and physical sciences, while reaching out to other disciplines and to encourage and enable **industrial usage and collaboration.**





Who we are

The Academic and Research Computer Hosting Industry and Enterprise in the West of Scotland (ARCHIE-WeSt) was established in March 2012 by a **£1.6M award** from the EPSRC e-Infrastructure fund to establish a “Tier-2” regional centre of excellence in High Performance Computing (**HPC**).





Our Strategic Goals

- Provide a step-change in HPC resource ***availability and accessibility*** to expand research collaboration in the West of Scotland
- Catalyse new computational science and engineering research and ***knowledge exchange collaborations***
- ***Promote*** HPC capabilities to industry
- Provide ***HPC training*** including the use ***of state-of-the-art software***
- Work in ***partnership*** with national/regional enterprise organisations and other supercomputing centres
- ***Support and promote*** the highest standards of computational science and engineering research



Who we are



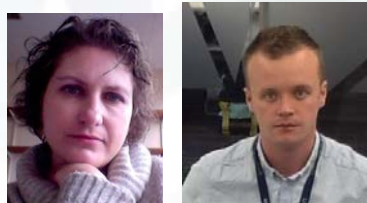
- **Associate Deputy Principal Prof. David Littlejohn**



- **Academic Director Prof. Maxim Fedorov**
- **Operational Director Dr Paul Mulheran**



- **HPC Manager Dr Richard Martin**
- **System Administrator Mr Jonathan Buzzard**



- **User Support Officer Dr Karina Kubiak – Ossowska**
- **Business Development Manager Dr Derek Bennet**

Our **International Advisory Board** includes Industrialists and Academics

We are committed to supporting Academia and Industry to exploit High Performance Computing, helping to **deliver projects efficiently and effectively.**



Our Service

- HPC at a **highly competitive price**
- **Free** introductory training and assistance
- **Priority service** for commercial customers
- Advanced training including: advanced HPC methods, Molecular Modelling (MD, MC, QM, QM/MM) and Chemo/Bio Informatics, Computational Fluid Dynamics, Finite Element Modelling, Visualisation, Audio/Video Signal Processing, Statistical Analysis and Data Mining, Optimization, Computational Physics, Computational Nanotechnology

Not for profit => excellent value for money



HPC vs desktop computer

Why HPC is “better” than a desktop computer:

- Some problems are simply too large for a desktop
- HPC has:
 - **More** cores
 - **More** RAM
 - **More** disk space
 - **Faster** read/write to disk

← **Most relevant to “Big Data”**



HPC vs own cluster

Why use ARCHIE-WeSt instead of buying your own cluster?

With your own cluster, total cost of ownership includes:

- Staff time is required to maintain the cluster
- Installing software
- Hardware maintenance issues
- Electricity cost
- Estates/cooling
- Maintenance costs

ARCHIE-WeSt is supported by **dedicated support team, vendor maintenance contracts, water cooled and housed** in a fully monitored machine room with UPS & generator backup.



Technical Specification

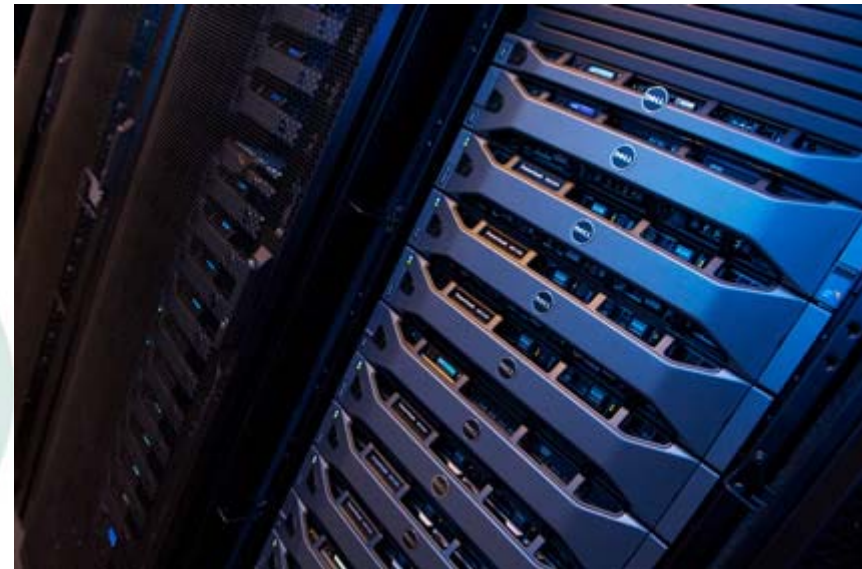
ARCHIE-WeSt is a state-of-the-art water cooled 38 Teraflop **HPC Facility** located at the University of Strathclyde

Standard Nodes:	3408 2.66GHz Intel Xeon X5650 cores (Westmere) 48GB RAM (4GB per core)
Large Memory Nodes:	Eight 512GB RAM nodes 2 Intel Xeon E7-4830 2.13GHz CPU's
GPU Nodes:	Eight Standard Nodes each with Nvidia Tesla M2075 GPU cards (448 cores, 6GB RAM)
Visualisation Nodes:	Two Dell R5500 servers with Nvidia Quadro 6000 graphics. 2 Xeon X5650 CPU's, 48GB RAM
Network:	QDR Infiniband 40GB/s networking throughout the whole cluster
Storage:	150TB of high performance LUSTRE parallel storage, capable of 3.5GB/s data transfer



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Technical Specification

- ARCHIE-WeSt uses the *Linux* operating system but also offers Windows virtual machine where is required
- It is possible to access ARCHIE-WeSt directly from a desktop computer using *Remote Desktop* software
- We promote the use of *Open Source* software and provide the access to many standard packages
- We also provide access to *Commercial Software* either under the terms of the user's own license or via short term license lease
- 9M core hours computation since July2012 (1050 “desktop years”)



HPC & Storage Performance

How does HPC assist Big Data projects?
Storage performance is critical

Verbatim Store 'n' Go review in External hard drives



[Gallery](#)

Verdict

Stick to the lower capacities and this is an unbeatable deal for a portable external hard disk

Review Date: 6 Oct 2011

Reviewed By: Darien Graham-Smith

Price when reviewed: £43 (£52 inc VAT)

Overall Rating

★★★★★

Features & Design

★★★★★

Value for Money

★★★★★

Performance

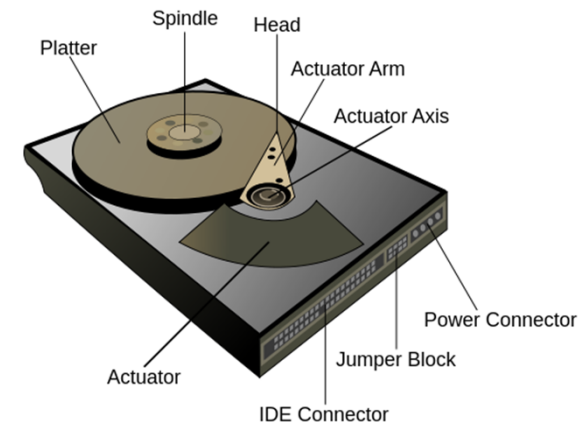
★★★★☆



Performance tests

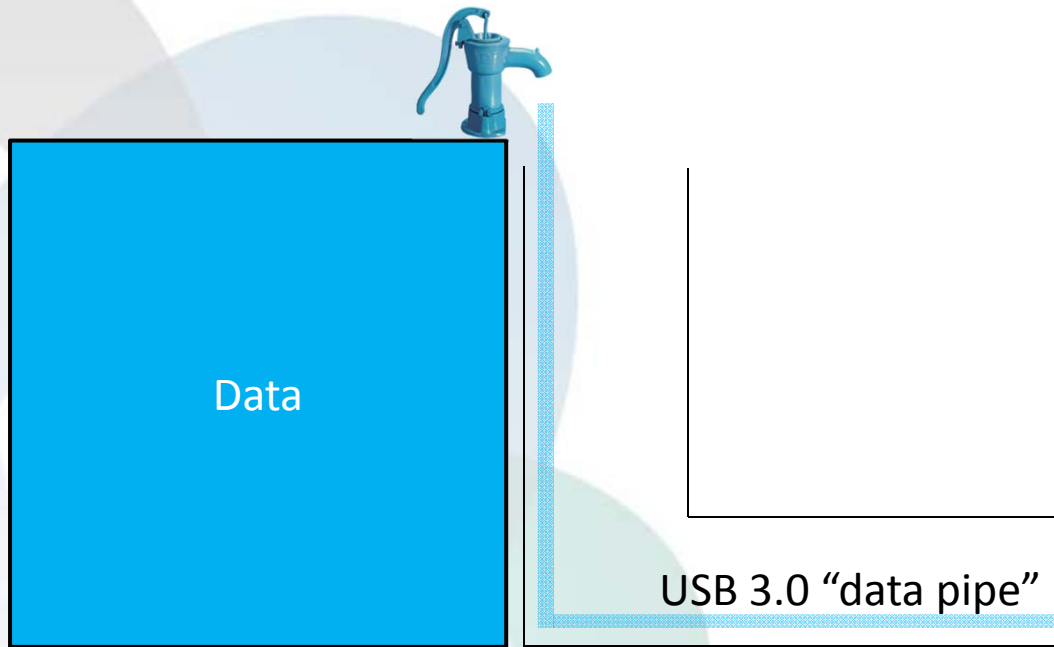
Write speed small files 51.0MB/sec

Write speed large files 82.0MB/sec



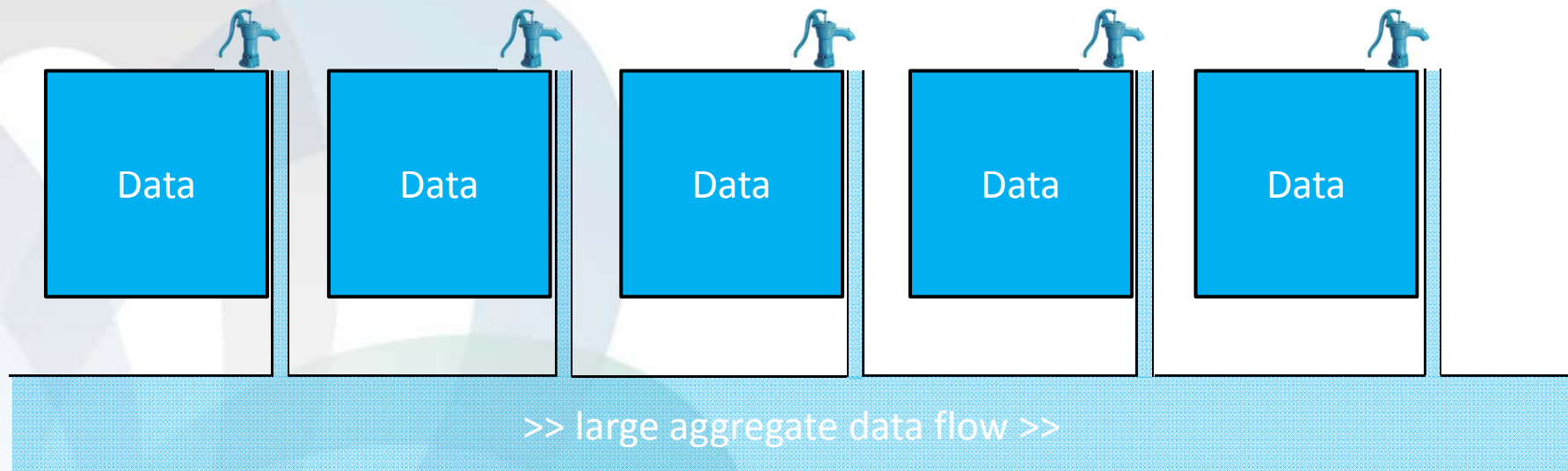


HPC & Storage Performance



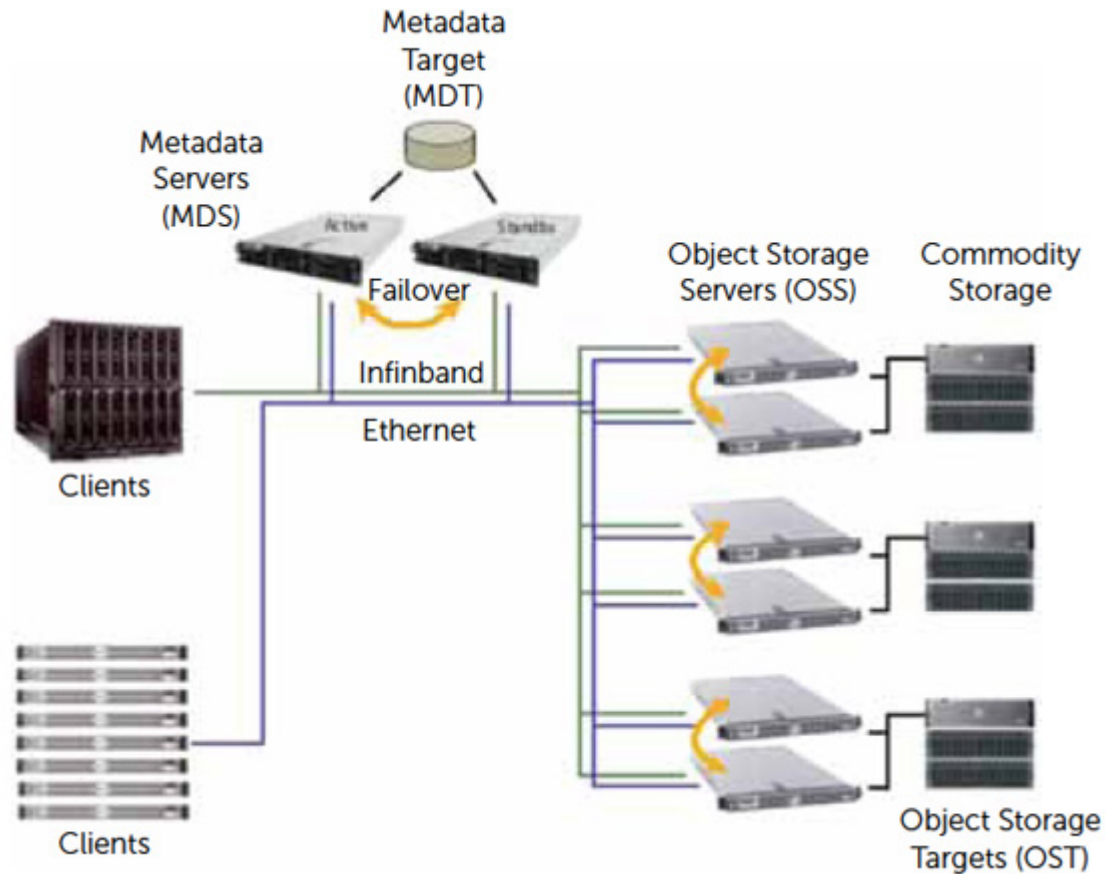


HPC & Storage Performance





HPC & Storage Performance



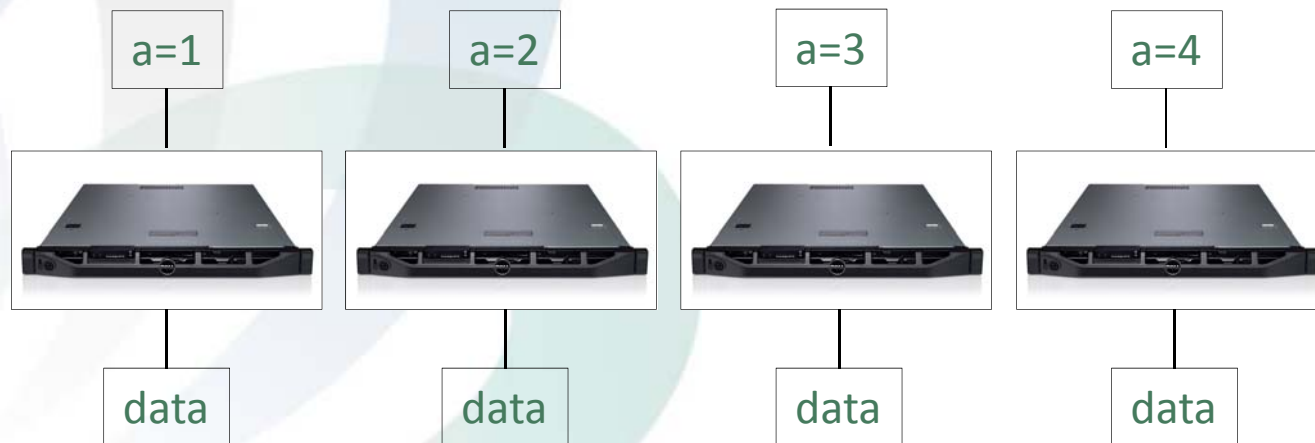
ARCHIE – WeSt : 3.5GB/s LUSTRE filesystem



HPC: Modes of Operation 1

1. Parameter Sweep

Repeat the same calculation on the same data many times for different input parameters

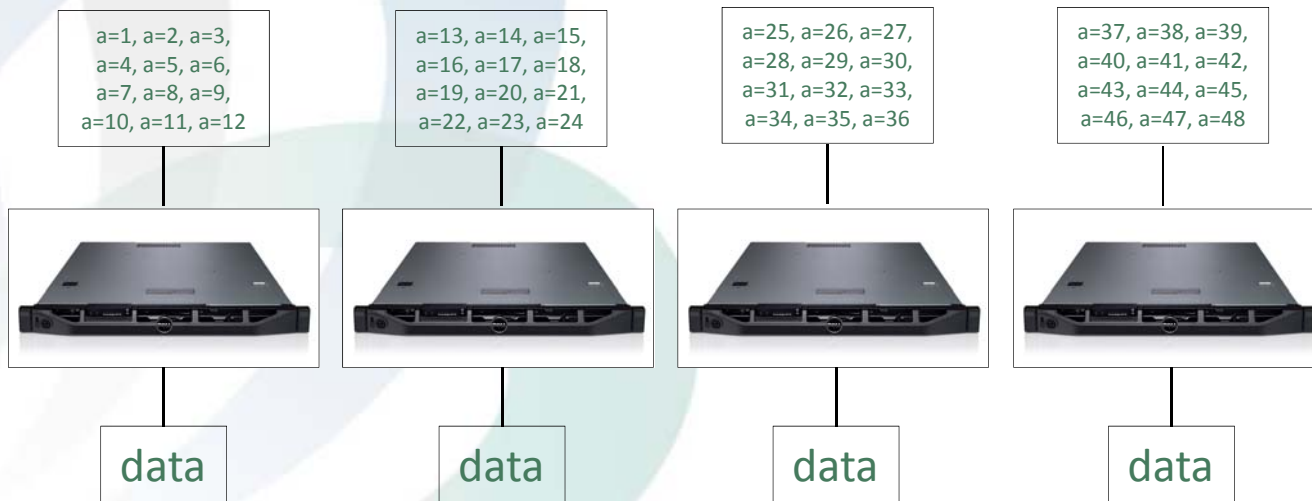




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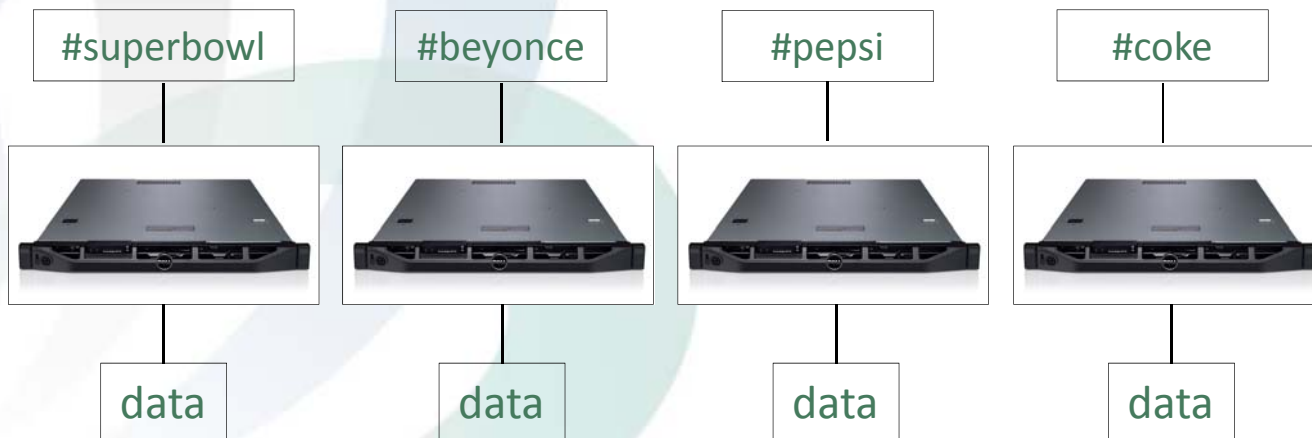




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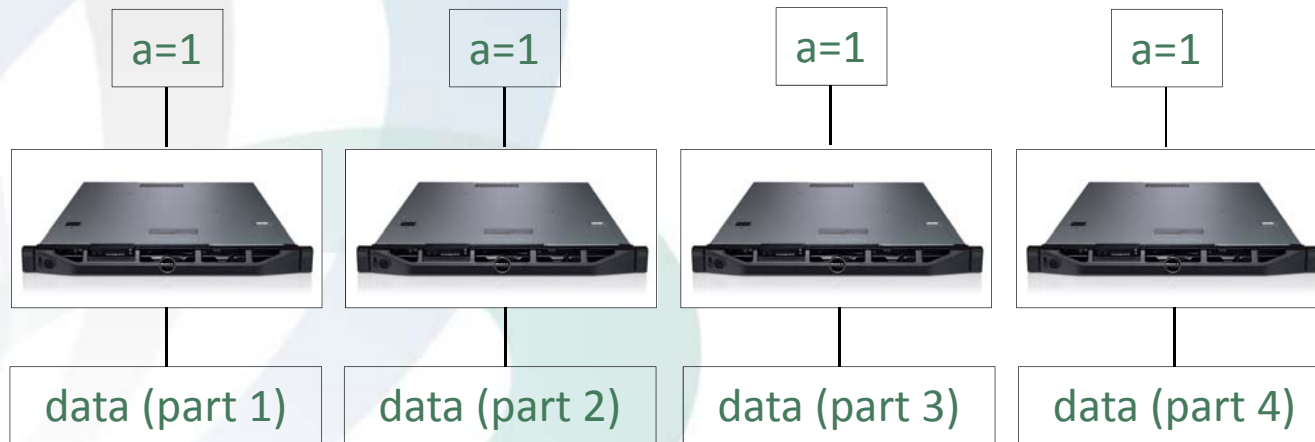




HPC: Modes of Operation 2

2. Distributed calculation

Repeat the same calculation on different portions of the data

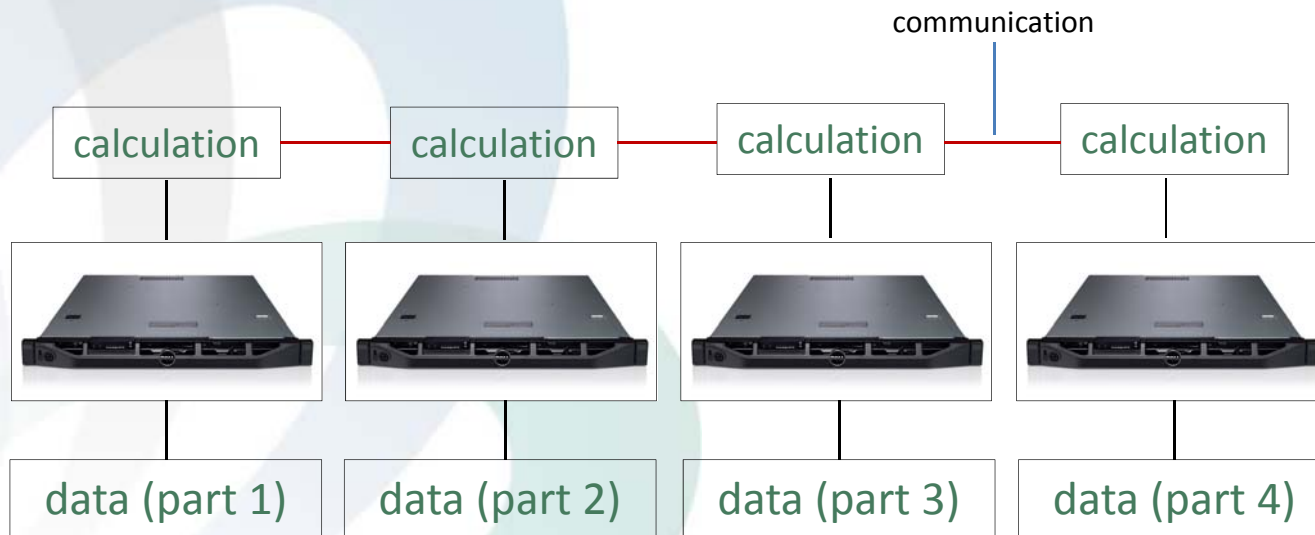




HPC: Modes of Operation 3

3. Parallel calculation

Perform one large calculation on different portions of the data





Software - examples

Open Source Software:

- **OpenFOAM** (computational fluid dynamics)
- **GROMACS, NAMD and VMD** (molecular dynamics)
- **Octave** (alternative to MATLAB)
- **ATLAS and R** (data analysis and statistical computing)
- **GCC** (Fortran, C and other compilers)
- **CUDA** (GPU programming)
- **AutoDock** (drug design)

Others can be installed on request



Software - examples

Commercial Software:

- **Intel Compiler Suite***
- **PGI Compiler Suite**
- **Ansys** (Finite element / Computational fluid dynamics)
- **Abaqus** (Finite element)
- **MATLAB** (Programming environment)
- **Comsol** (Multiphysics software)
- **Schrodinger** (Computational drug design)
- **ADF** (Density Functional Theory Modeling Suite)

Others can be installed on request *(subject to licensing terms)*



Summary

HPC provides the necessary performance for Big Data projects

- **ARCHIE-WeSt provide both resources and support**
- **New users are fully supported to get up and running**
- **We assist people migrating to our service**
- **ARCHIE-WeSt provides high-end computational resources**
- **ARCHIE-WeSt provides a competitive advantage**
- **ARCHIE-WeSt fosters collaborations with industry**



Final Remarks

Contact us: www.archie-west.ac.uk

To apply: <http://www.archie-west.ac.uk/apply/archie-application-form>
<http://www.archie-west.ac.uk/apply/non-academic-users>

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For commercial enquiries, please contact:

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ARCHIE-WeSt

Thank you for your attention