High End Computing at Cardiff University
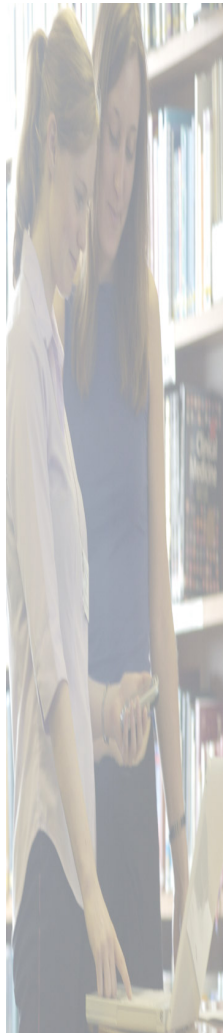
Focus on Campus Grids

James Osborne

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- High End Computing Spectrum
- Facilities at Cardiff
- Condor at Cardiff
- Success Stories
- High End Computing Futures
- Questions

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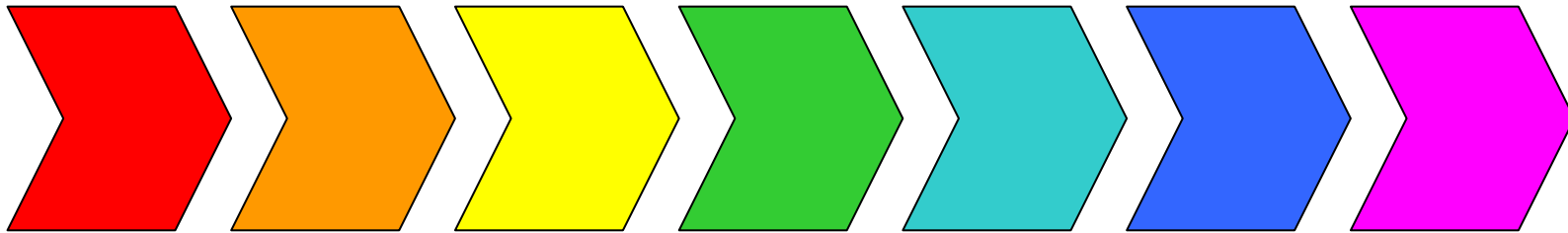
High End Computing Spectrum

The HEC Spectrum

HPC

Tightly Coupled

HTC

Loosely Coupled

Supercomputers

NUMA Machines

£ Million+

Large Clusters

SMP

£ H Thousand

£ Million
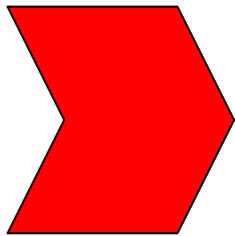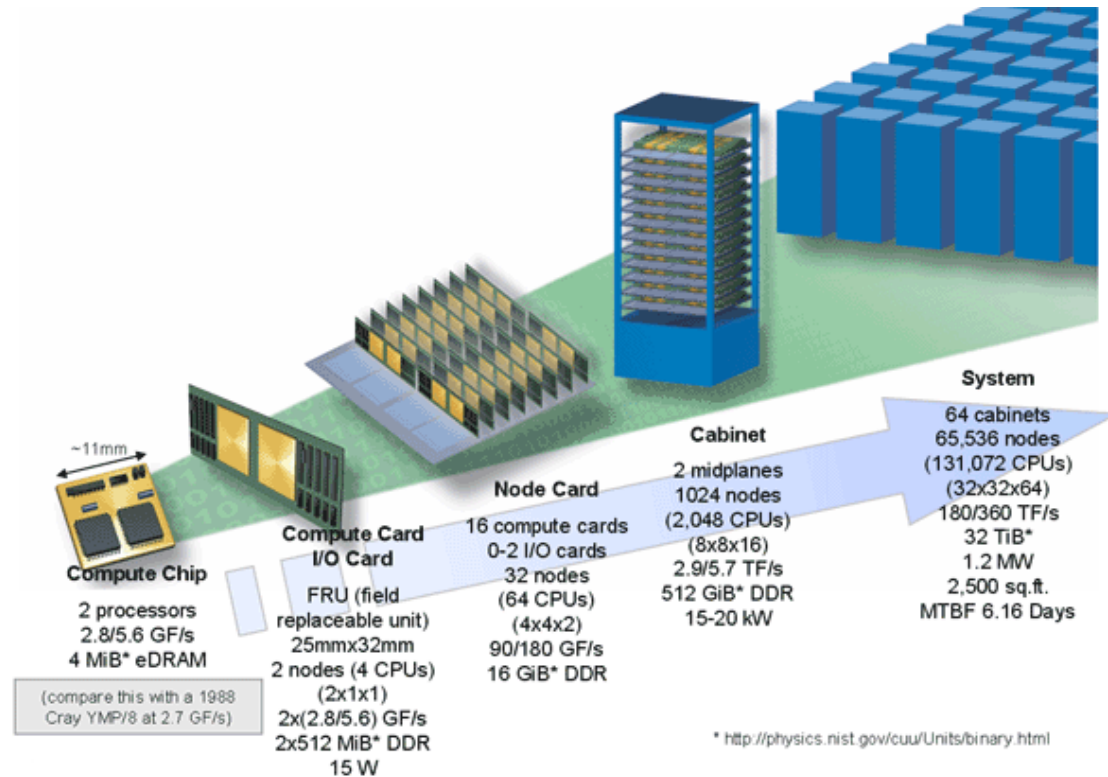
Small Clusters

Campus Grids

£ Thousand

£ H Thousand

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The HPC End

HPC

Tightly Coupled

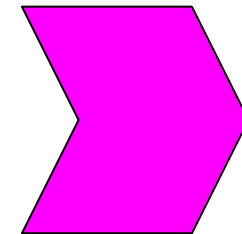Supercomputers
Bluegene L
131,072 CPUs

~11mm

Compute Chip

2 processors
2.8/5.6 GF/s
4 MiB* eDRAM

(compare this with a 1988
Cray YMP/8 at 2.7 GF/s)

**Compute Card
I/O Card**

FRU (field
replaceable unit)
25mmx32mm
2 nodes (4 CPUs)
(2x1x1)
2x(2.8/5.6) GF/s
2x512 MiB* DDR
15 W

Node Card

16 compute cards
0-2 I/O cards
32 nodes
(64 CPUs)
(4x4x2)
90/180 GF/s
16 GiB* DDR

Cabinet

2 midplanes
1024 nodes
(2,048 CPUs)
(8x8x16)
2.9/5.7 TF/s
512 GiB* DDR
15-20 kW

System

64 cabinets
65,536 nodes
(131,072 CPUs)
(32x32x64)
180/360 TF/s
32 TiB*
1.2 MW
2,500 sq.ft.
MTBF 6.16 Days

* http://physics.nist.gov/cuu/Units/binary.html

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The HTC End

HTC
Loosely Coupled

Campus Grids
Condor@Cardiff
600+ CPUs

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Facilities at Cardiff

Facilities at Cardiff - Helix

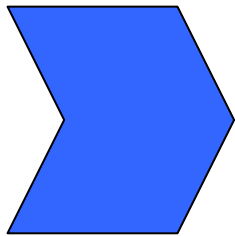Large Clusters

Helix

200 CPUs

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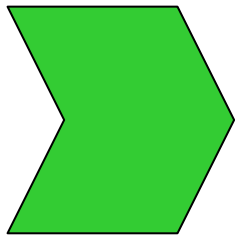
Facilities at Cardiff - SGI

Small Clusters

SGI Origin 300
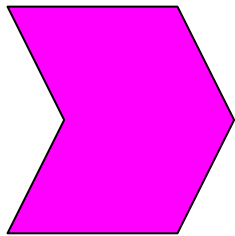
32 CPUs

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Facilities at Cardiff - Condor

Campus Grids

Condor@Cardiff

600+ CPUs

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Condor at Cardiff

What is Condor ?

- Condor is a software system that creates a High-Throughput Computing (HTC) environment

- Condor effectively utilizes the computing power of workstations that communicate over a network

- Condor's power comes from the ability to effectively harness resources under distributed ownership

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What is a Condor Pool ?

- A pool is a collection of workstations that communicate over a network
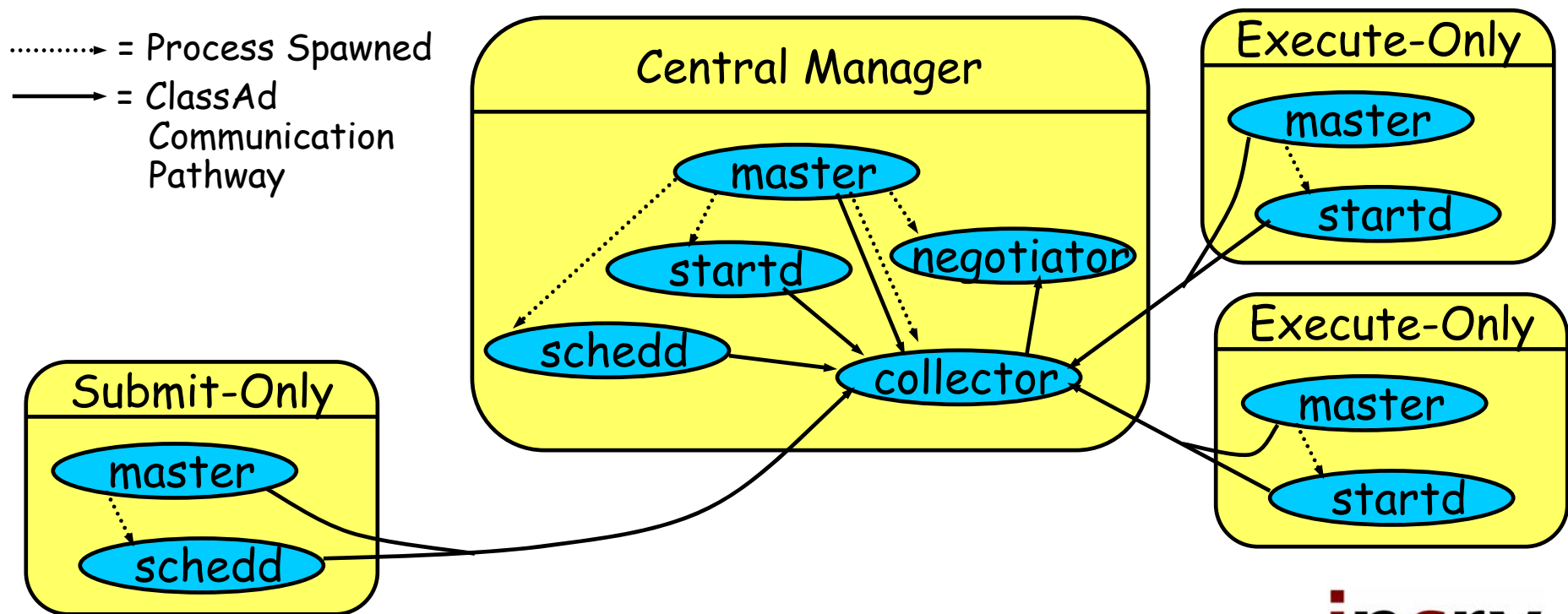
What is a Condor Job ?

- A command line windows executable
  - ▶ All files in a self-contained directory structure
  - ▶ Condor runs jobs in a sandbox *..\execute\...*
  - ▶ Condor runs jobs as user *condor-reuse-vm1*
- One or more input files
- One or more output files
- A submit script
  - ▶ One or more logs – useful for debugging

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What Goes In A Submit Script ?

- **Running myprog 100 times**

  universe = vanilla

  executable = myprog.exe

  input = myin.$(PROCESS)

  output = myout.$(PROCESS)

  error = myerr.$(PROCESS)

  queue 100

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What Else Can Go In ?

root_dir = c:\mydirectory

transfer_files = ALWAYS

transfer_input_files = $(ROOT_DIR)\afile.txt

transfer_output_files = $(ROOT_DIR)\afile.txt

log = mylog.$(PROCESS)

notification = NEVER | ERROR

arguments = -arg1 -arg2

What Else Can Go In ?

requirements =

    OpSys == "WINNT51"

    Machine == "hostname.cf.ac.uk"

How Do I Submit A Job ?

- In the first instance by sending all your files to condor@cardiff.ac.uk to allow us to tailor your jobs to our environment

- In time by seeking permission to submit your own jobs to condor@cardiff.ac.uk to allow us to enable your workstation as a submit host
  - ▶ Currently requires IP address change

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How Do I Submit A Job ?

- Submitting your job

  `condor_submit myscript.sub`

- Checking your job's progress

  `condor_q`

- Checking the pool

  `condor_status`

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Terms of Use

- Any local researcher can use the campus grid on the proviso that they…
  - write a short summary of their research that we can use to publicise their use of the campus grid
  - provide references to journal articles and conference proceedings containing appropriate acknowledgements

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Success Stories

Prof Tim Wess

- OPTOM
- X-Ray Diffraction
- Determine shape of molecules
- Time on a single workstation = 2-3 Days
- Time on the campus grid = 2-3 Hours
- Speed-up factor of ~20

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Prof Tim Wess

- "This capability provides the final link in the chain that Cardiff has established to solve macromolecular structures"

- "Our involvement with synchrotron sources such as DIAMOND … and the residence of CCP 13 … ensures that we are well placed to be in the vanguard of structure determination"

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Soyeon Lee

- CARBS
- Montecarlo Simulation
- 20,000 parameters for 90 different models
- Time on a single workstation = 42 Days
- Time on the campus grid = 2 Days
- Speed-up factor of ~20

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Dr Kevin Ashelford

- BIOSI
- Distributed Search
- Identify corrupt records in a DNA database
- Time on a single workstation = 2.4 Years
- Time on the campus grid = 2.6 Weeks
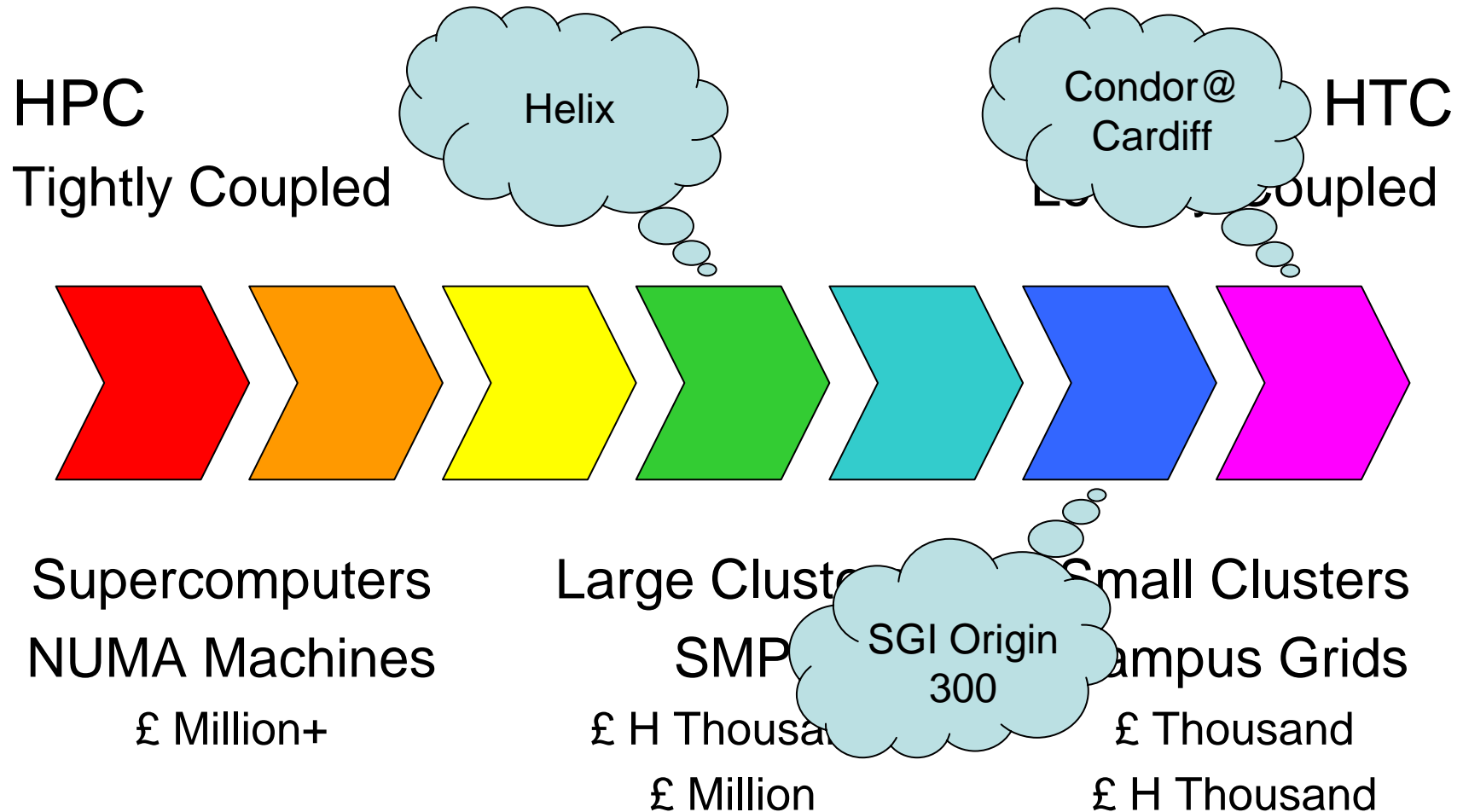- Speed-up factor of ~50

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Dr Kevin Ashelford

- "This is a significant contribution to microbial research and will hopefully be the required impetus for the world-wide research community to improve current methods"
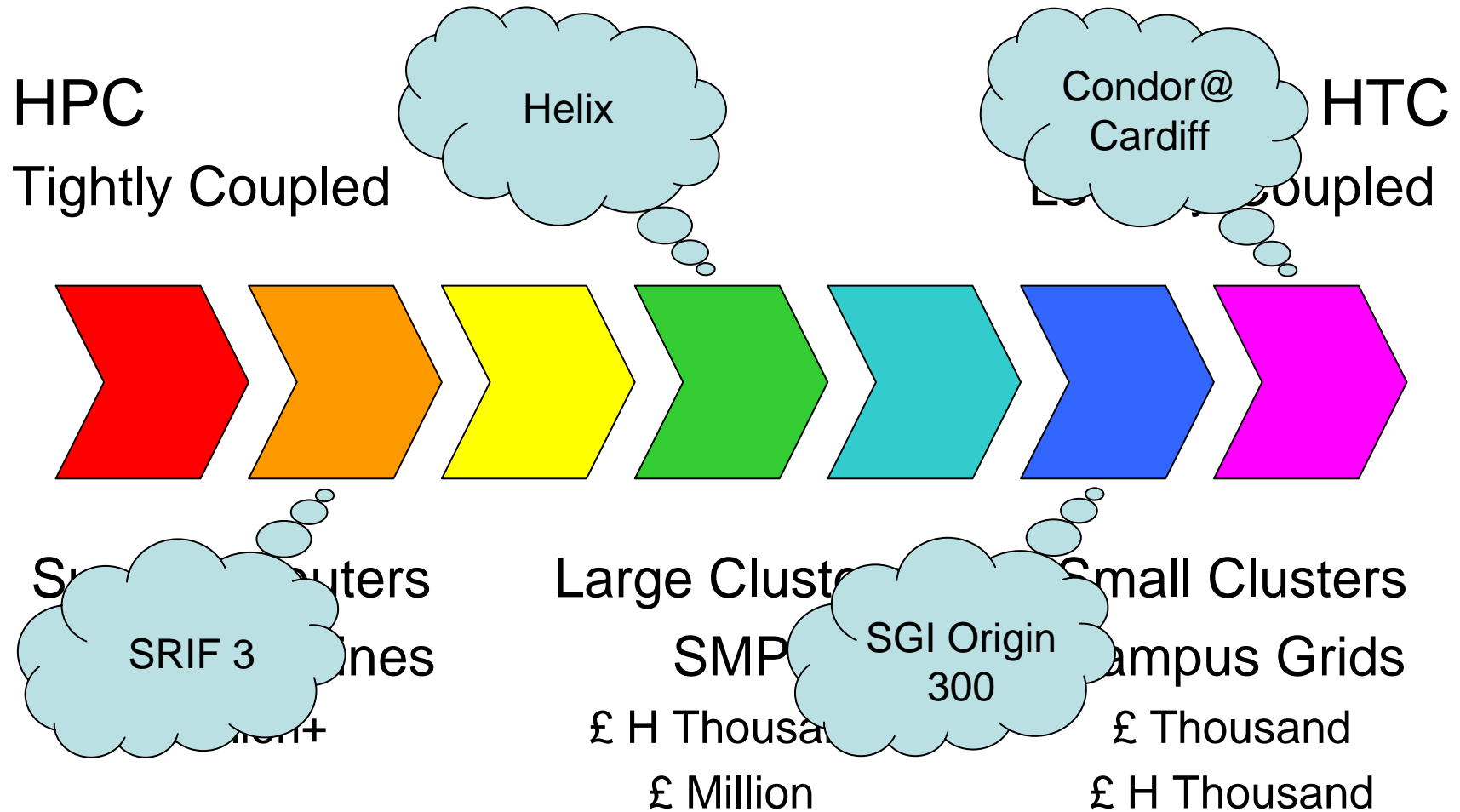
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High End Computing Futures

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Questions ?

condor@cardiff.ac.uk