

Science & Technology
Facilities Council



The Octopus SCARF

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Science & Technology Facilities Council

Rutherford Appleton Laboratory

UK Research & Innovation

<https://stfc.ukri.org>

UK Research and Innovation

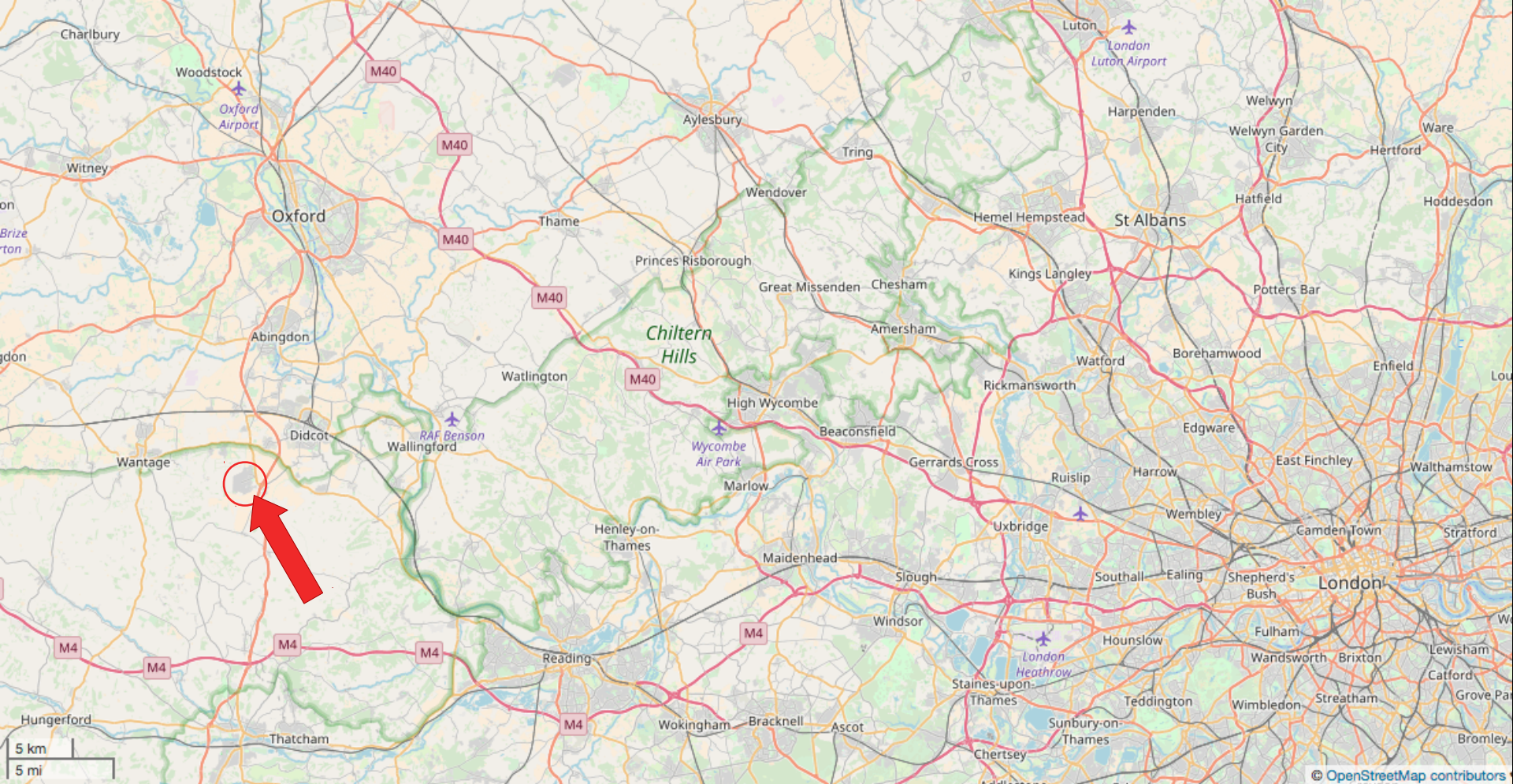
- Seven Research councils:
 - Arts and Humanities Research Council
 - Biotechnology and Biological Sciences Research Council
 - Economic and Social Research Council
 - Engineering and Physical Sciences Research Council
 - Medical Research Council
 - Natural Environment Research Council (Boaty McBoat Face)
 - **Science and Technology Facilities Council**
- Other councils:
 - Innovate UK
 - Research England



STFC

- Research and Grants
 - Astronomy
 - Particle Physics
 - Nuclear Physics
 - Space Science
- National Labs
 - Daresbury Laboratory, Cheshire
 - **Rutherford Appleton Laboratory, Harwell, Oxfordshire**





European HTCondor Workshop

Tuesday Sept 4th through Friday Sept 7th
More details and registration coming soon!



GridPP WLCG Tier1

~22000 slot HTCondor pool

~13PB disk storage in Ceph

~16PB disk storage in CASTOR

>30PB tape storage in CASTOR

<https://www.scd.stfc.ac.uk>



Diamond Light Source

3 GeV, 3rd Gen Light Source
~40 beamlines

X-ray to far-infrared radiation

<http://diamond.ac.uk>



ISIS Neutron & Muon Source

800MeV Proton accelerator
Tungsten targets → Neutrons
Graphite targets → Muons
+ MICE experiment

<https://www.isis.stfc.ac.uk>



RAL Space

Space research and
technology development

210 space missions (incl. JWST)

<https://www.ralspace.stfc.ac.uk>



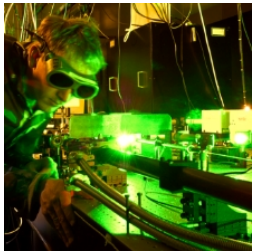
Central Laser Facility

Wide array of lasers for vast range of scientific applications

<https://www.clf.stfc.ac.uk>

Central Laser Facility

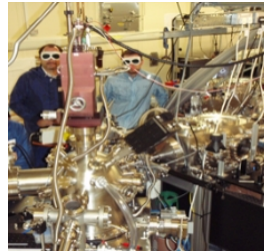
ASTRA GEMINI



VULCAN



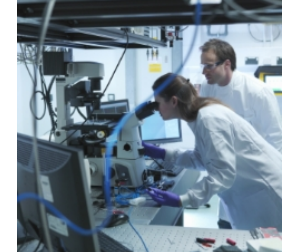
ARTEMIS



ULTRA



OCTOPUS



High-power, ultra-intense lasers for extreme conditions science & applications

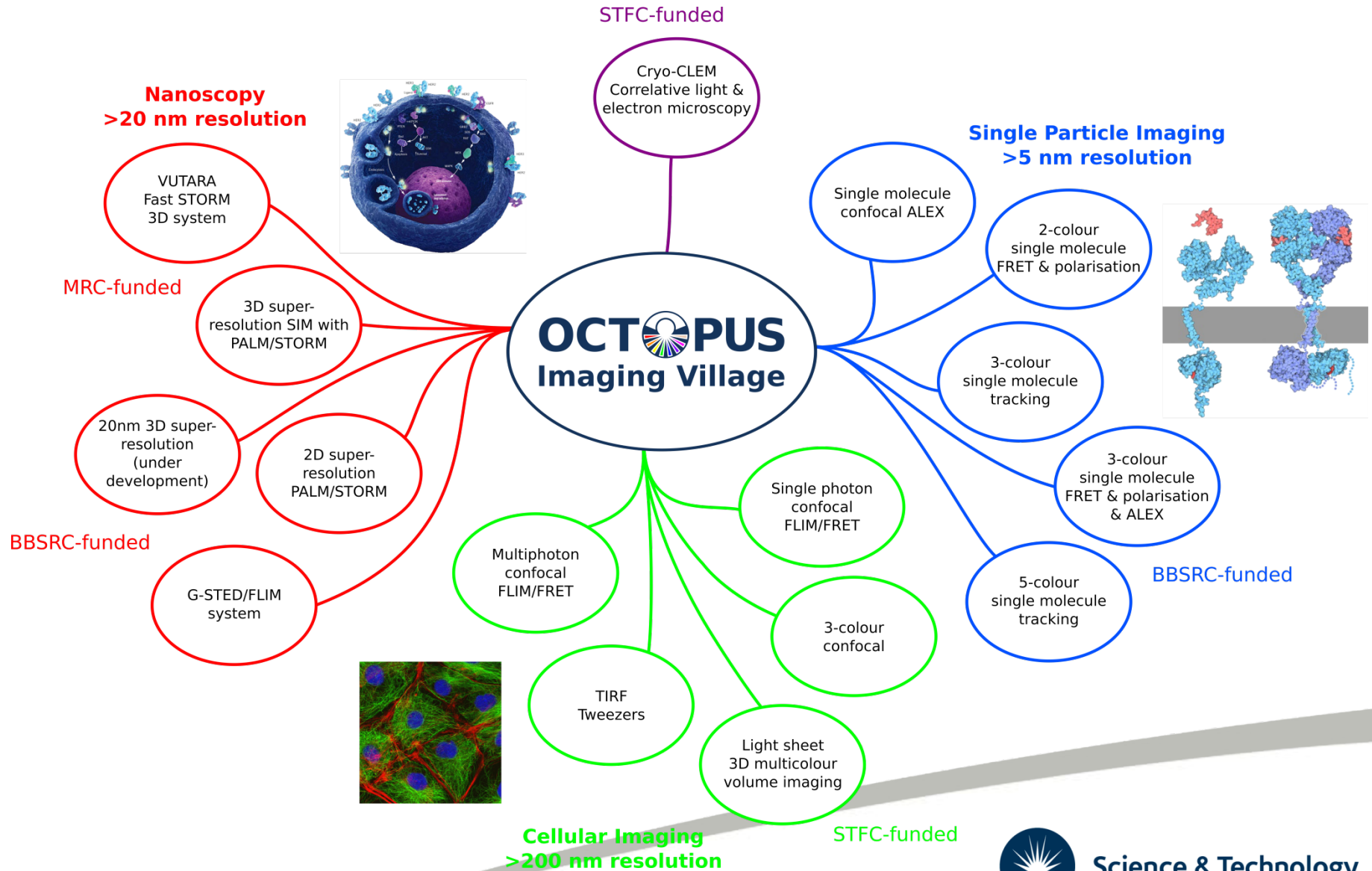
Laser applications in the physical and life sciences (materials, chemistry, biology)



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OCTOPUS



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- National imaging facility with peer-reviewed, funded access
- Located in Research Complex at Harwell
- Cluster of microscopes and lasers and expert end-to-end multidisciplinary support
- Computing is predominantly a middleware challenge
 - “Looking forward to hardware bottleneck”



SCARF

- HPC cluster open to all STFC departments and Diamond to support scientists and researchers
 - ~700 nodes
 - ~14000 cores
 - ~52TB RAM
 - Infiniband interconnect
- Twenty-four nodes with GPUs
 - 12 with dual K40s (reserved for OCTOPUS)
 - 12 with dual K80s (free for all)

<http://www.scarf.rl.ac.uk>



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Octopus Data

- Catalogued in ICAT <https://icatproject.org>
- Browsed with TopCAT
- Jobs can run against data using the ICAT Job Portal



ICAT Job Portal

The screenshot displays the ICAT Job Portal interface, which is a web-based application for managing and analyzing microscopy data. The interface is divided into two main sections: a search results page on the left and a detailed view of a specific dataset on the right.

Search Results Page (Left):

- Filters:** The top section contains filters for 'Any users', 'Any instrument' (Unknown instrument, OctopusSM2), 'Any experiment type' (Unknown experiment type, Colocalisation), and 'Any number of channels' (1 channel, 3 channels).
- Search Results:** A table lists three projects found. The first project is selected, showing its details in a table below.

Dataset Details Table:

Dataset ID	ProjectName	comments	experiment_type	instrument	nchannels	nframes	sampledescription	users	Created	Done
4454	20120525_0004_0001_6e28e0b5-fe99-45a4-93d7-61a952a35912		Colocalisation	OctopusSM3	3	601	coloc 3 Affibodys T47D		2012-10-23T12:53:13+01:00	2012-10-23T13:01:22+01:00

Detailed View (Right):

- FrameViewer:** Displays three channels of microscopy data: (R) 1: Atto_647N (ColocalisationTarget), 2: Alexa546 (ColocalisationTarget), and 3: Alexa488 (ColocalisationTarget). The image shows a grid of cells with colored spots.
- TraceViewer:** Displays a line graph of the signal intensity over time (0 to 600 seconds). The graph shows a sharp increase in signal around 150 seconds, followed by a plateau. A histogram on the right shows the frequency distribution of the signal intensity.
- Messages:** Displays a list of messages related to the dataset, including the file name and the user who created it.

ICAT Job Portal

- Frontend for pre-defined analysis against datasets
- Written in Java
- Originally designed for direct submission
 - Connectors for Torque and LSF
 - Now need HTCondor, Slurm and OpenStack.
- DAaaS project called for a compute broker
 - Standardised interface for submission
 - Onward submission to batch farms and clouds
 - Sounds like HTCondor!

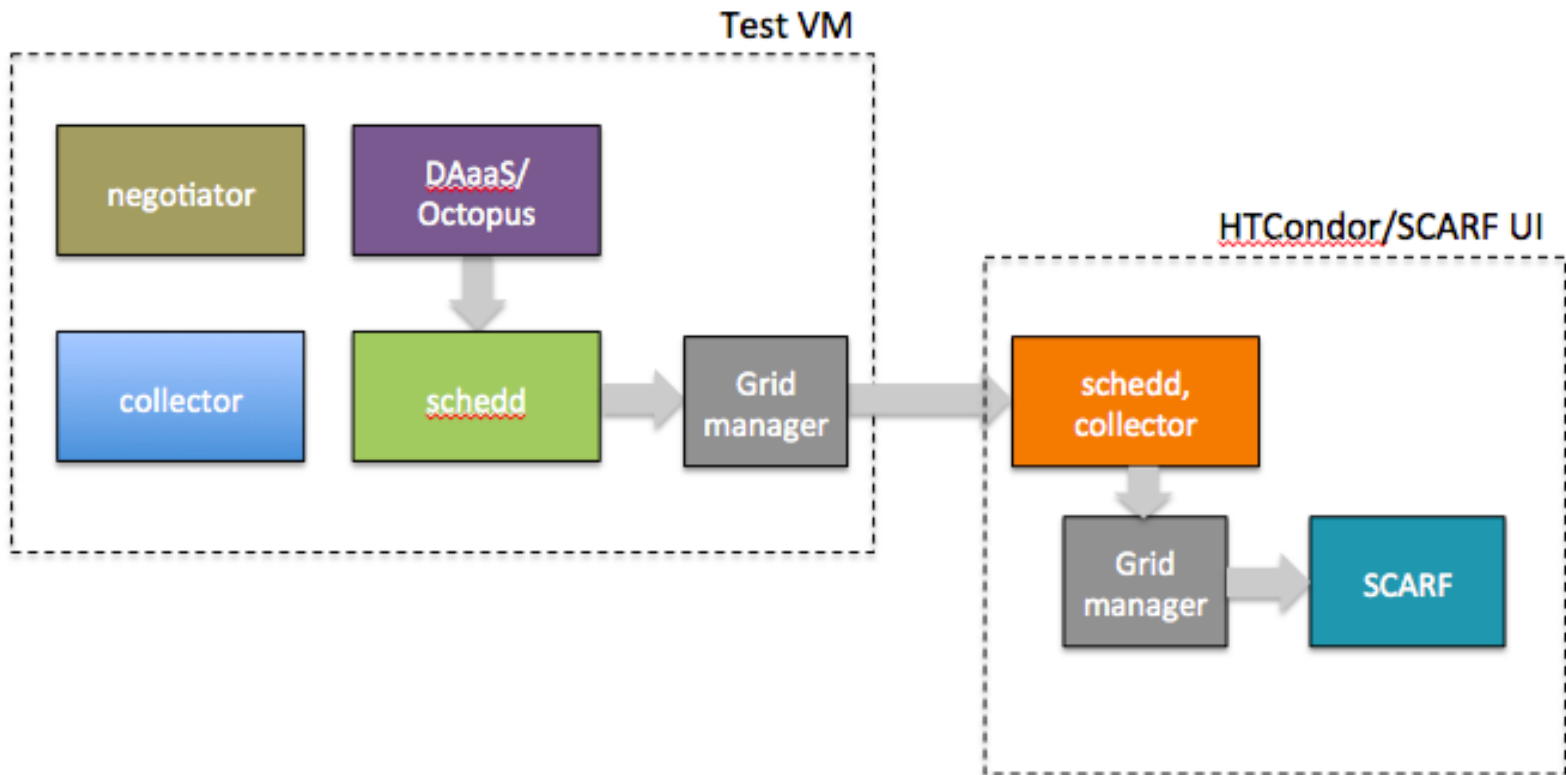


Compute Broker

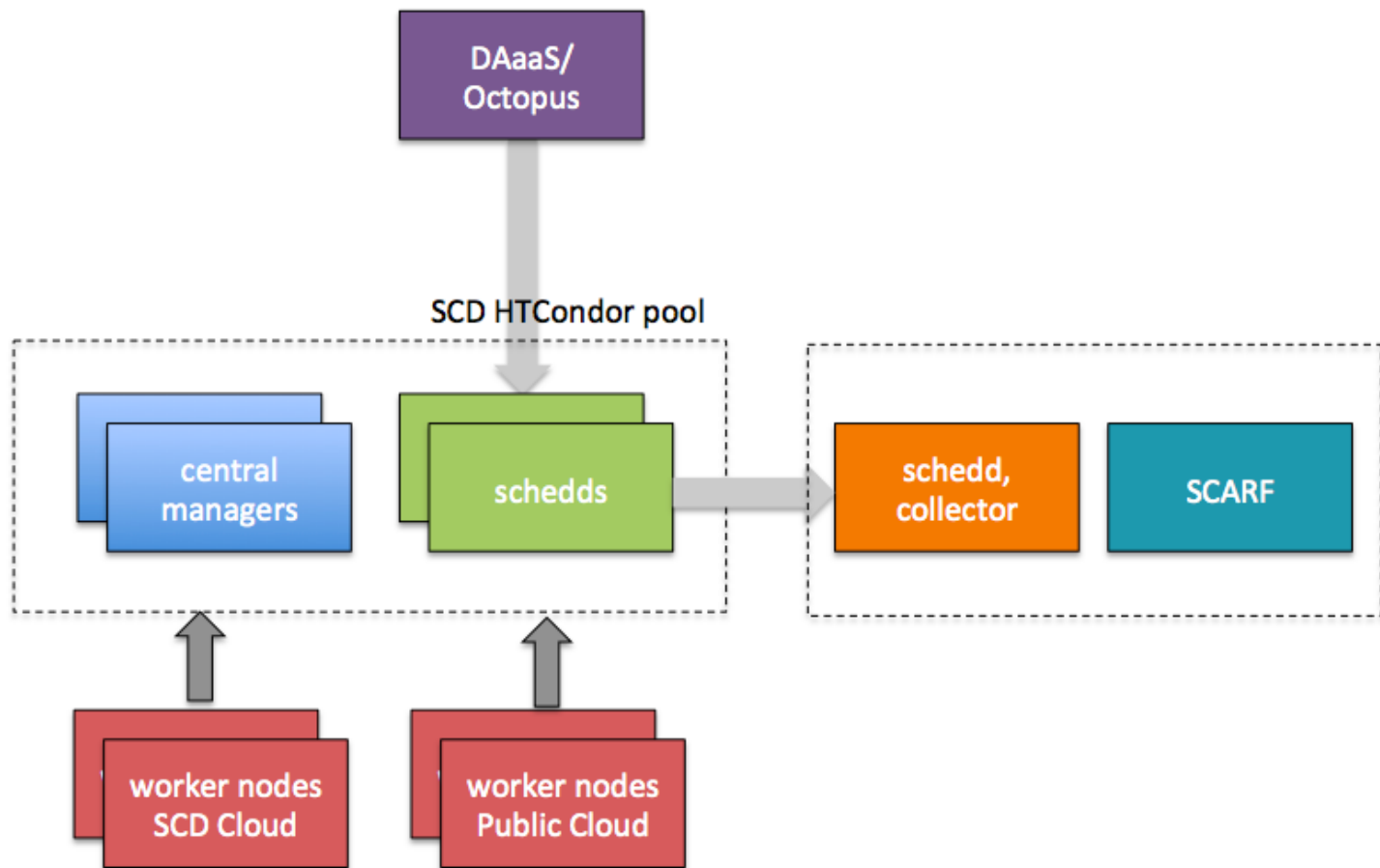
- Essentially HTCondor-CE
 - Grid Universe
 - Some user translation “magic” for SCARF
 - Jobs get wrapped and use Singularity on SCARF



Right now...



Eventually..?



Questions!

- Users want feedback from jobs
 - Want to see progress while running
 - Difficult to inspect job from outside
 - Tried side-channel access
 - Considering pilot jobs
- Any suggestions?

