# 12 years of iRODS at Sanger: *What we've learned and what's next*

iRODS UGM Wellcome Sanger Institute 2021

Peter Clapham

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# Who are we ?

Genome research Campus ~ 10 miles south of Cambridge (UK)

Established 1992

Part of the world wide human genome project

*https://www.sanger.ac.uk/about/who-we-are/history-of-the-sanger-institute/*

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# Science doesn’t stand still

Nature draft of the first human genome 2001

: https://www.nature.com/articles/35057062

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# The ~~Solexa~~ Illumina sequencers were arriving !

Second generation sequencers.

Massive parallelisation meets sequencing.

*https://www.enterprise.cam.ac.uk/case-studies/solexa-second-generation-genetic-sequencing/*

Huge potential for increasing the speed, capacity and sequencing scale that could be delivered.

In 2015 it was possible to sequence a human genome for $1000 / sample in ~1 day vs 10 years and £10M on across a world wide consortium

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# One good idea, and a little innovation led to

*https://www.ch.cam.ac.uk/collaboration-and-impact/solexa-sequencing*

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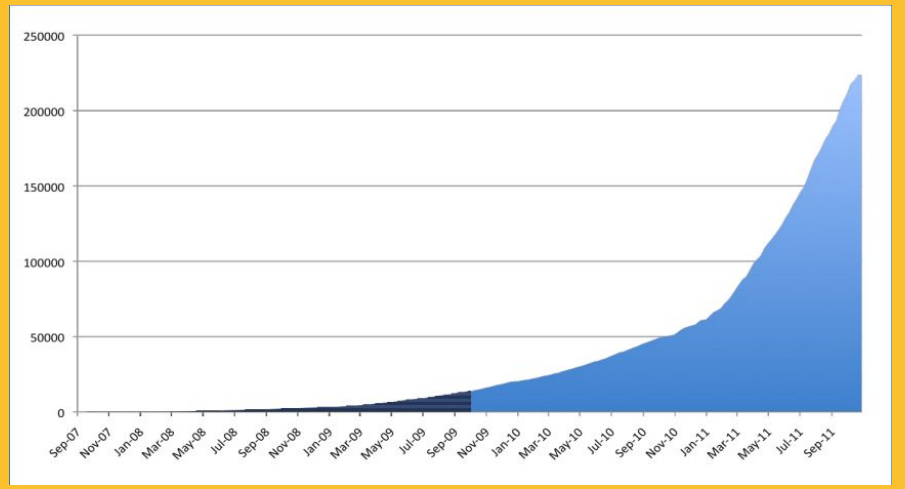
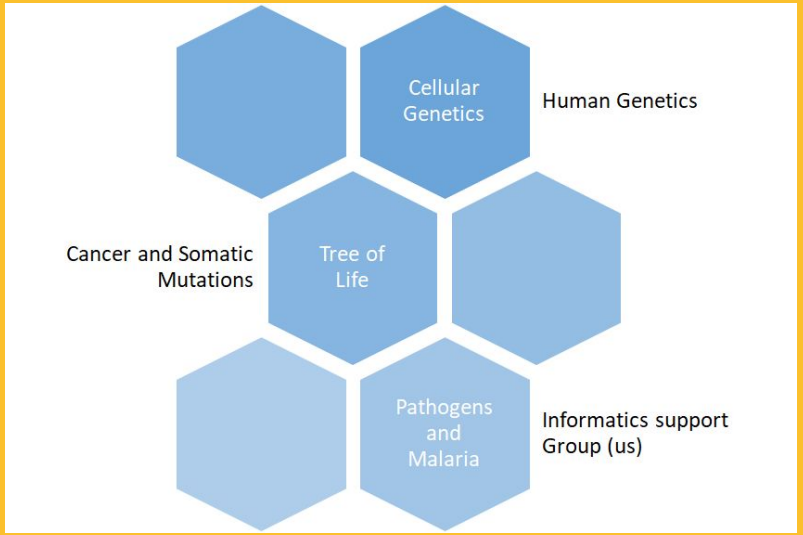
# New tech drove “massive data growth”



# New technology: new opportunities



# So how are we going to manage this data ?!

Weekly calls with the Broad tech teams.

“So how many Sun Thumpers do you have next to the sequencers at the moment ?”

We had a system in place, that worked, but it was handcrafted and scale was becoming an issue

How should we be searching for our data ?

How should data be organised ?

***What does good look like ?***

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# What had we learned up to this point ?

- Finding data can be hard
- Managing data can be hard
- We need something that will scale
- We need a tool / service that manages the data and does not become its own monster

KISS !

Think about a plan B

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# Options ?

In early 2009 / 2010 not too many options available.

Dcache
SRM / SRB
General Atomics (Nirvana)
iRODS ?

Mostly out of the High energy Physics world.
***Very helpful people !***

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# So why iRODS ?

## Where’s my data ?!

Managed data delivery and curation.

Defined data workflows.

Strong iRODS rule engine.

Hardware agnostic.

Data lives on disk, meta-data in a database.

Checks for data status at rest.

No *cul de sacs*

*NEW SEQ TECH INCOMING !*

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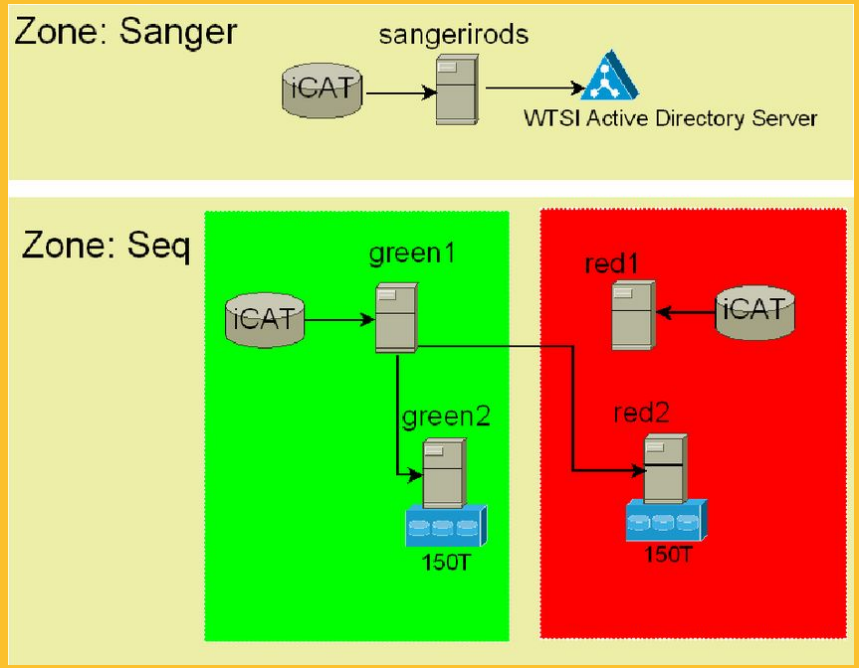
# Version 1.0

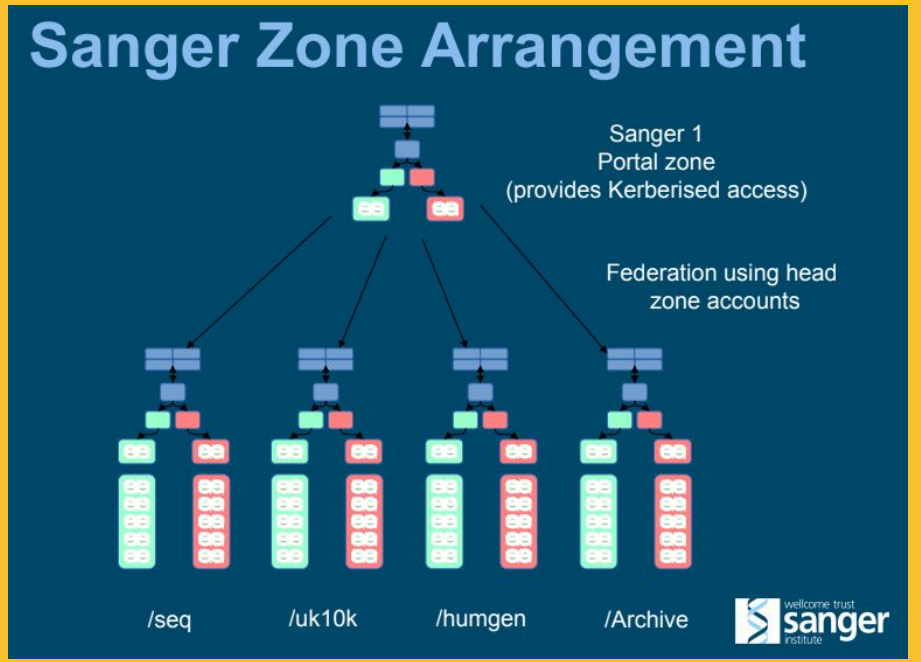
Our first release was described here:

https://www.researchgate.net/publication/51637790_Implementing_a_genomic_data_management_system_using_iRODS_in_the_Wellcome_Trust_Sanger_Institute



# Things then developed pretty fast..

iRODS UGM 2015

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# Meta-data became really important

Structured data-curation

Example attribute fileds →

Users query and access data largely from local compute clusters

Users access iRODS locally via the cli

attribute: library
attribute: total_reads
attribute: type
attribute: lane
attribute: is_paired_read
attribute: study_accession_number
attribute: library_id
attribute: sample_accession_number
attribute: sample_public_name
attribute: manual_qc
attribute: tag
attribute: sample_common_name
attribute: md5
attribute: tag_index
attribute: study_title
attribute: study_id
attribute: reference
attribute: sample
attribute: target
attribute: sample_id
attribute: id_run
attribute: study
attribute: alignment

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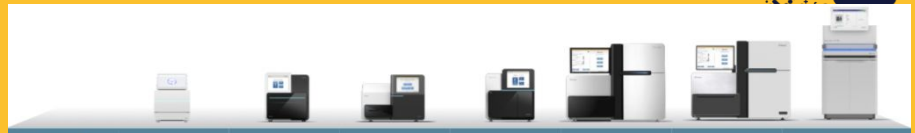
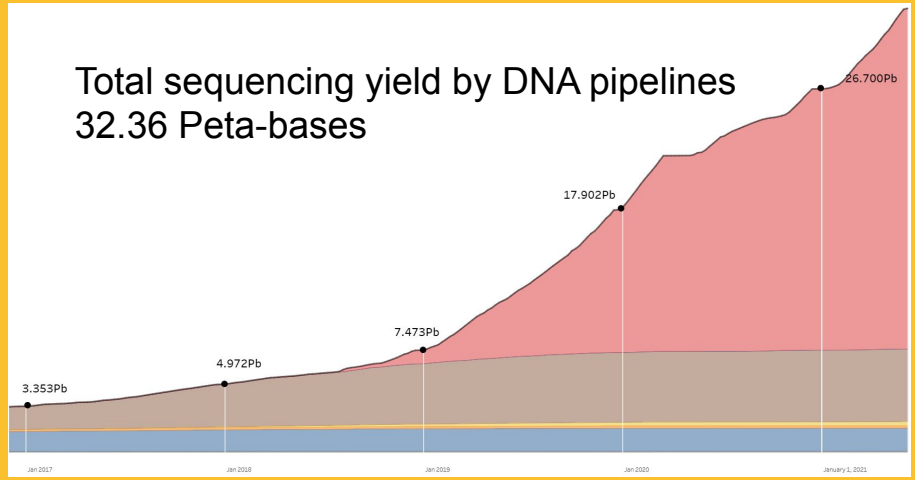
# Today

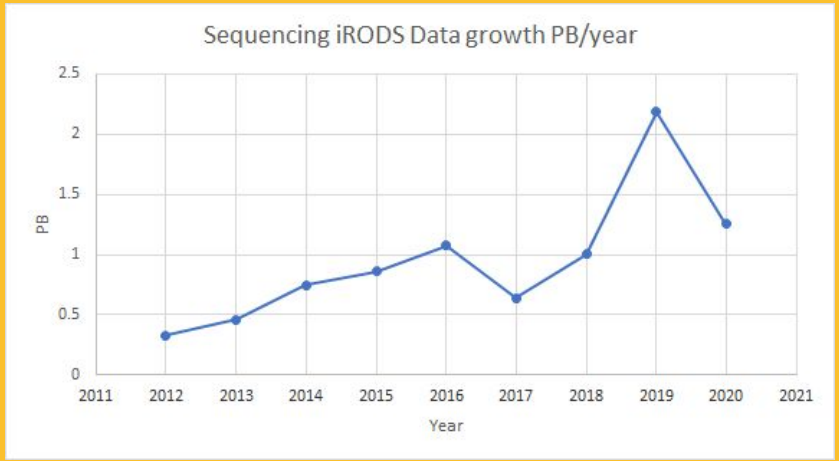


| Sequencing System | iSeq™ | MiniSeq™ | MiSeq® | NextSeq® | HiSeq® | HiSeq® X | NovaSeq® |
|---|---|---|---|---|---|---|---|
| | | | | | 4000 | Five/Ten | 6000 |
| **Output per run** | 1.2 Gb | 7.5 Gb | 15 Gb | 120 Gb | 1.5 Tb | 1.8 Tb | 1 Tb - 6 Tb[1] |
| **Instrument price** | $19.9K | $49.5K | $99K | $275K | $900K | $6M[2]/$10M[2] | $985K |
| **Installed base**[3] | NA | ~600 | ~6,000 | ~2,400 | ~2,300[4] | | ~285 |




https://www.illumina.com/content/dam/illumina-marketing/documents/products/illumina_sequencing_introduction.pdf

# Which in iRODS translates to




*If 2021 had matched 2020, ~40% of the data in the archive would be < 2 years of age.*

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# Data under control, sort of

Automated data replication

Managed metadata

New tools to manage data ingress at scale, Baton, tears

BUT there are some challenges

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# Eventually scale hurts

- Meta-data searches become slow.
- An expectation for a strong GUI interface
- Ensuring rules are run effectively across all zones
- Managing many small systems is OK IF THEY ARE ALL THE SAME.
- Build systems change
- Upgrades and roll outs slow
- Risk that the data beast takes charge !

***See John Constable's talk on tech debt later.***

***Did we keep it simple ?***

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# And the world is changing too

- **Politically**, UK no longer a part of europe
- New **economic** opportunities, UKB
- **Social**, COVID has hit us all, vaccines, fake news, who do I / you believe ?
- **Technology** bringing more opportunities daily, Oxford Nanopore ? Real time sequencing ?
- **Environmental** impacts, and dealing with compute at peta and exascale ?

LEGAL !!

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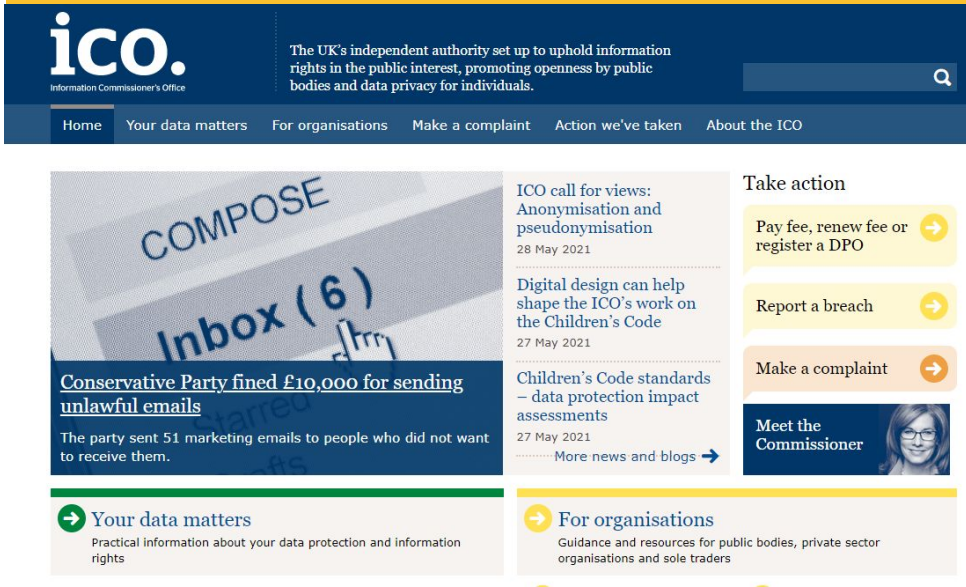
# GDPR and Data governance Needs YOU !

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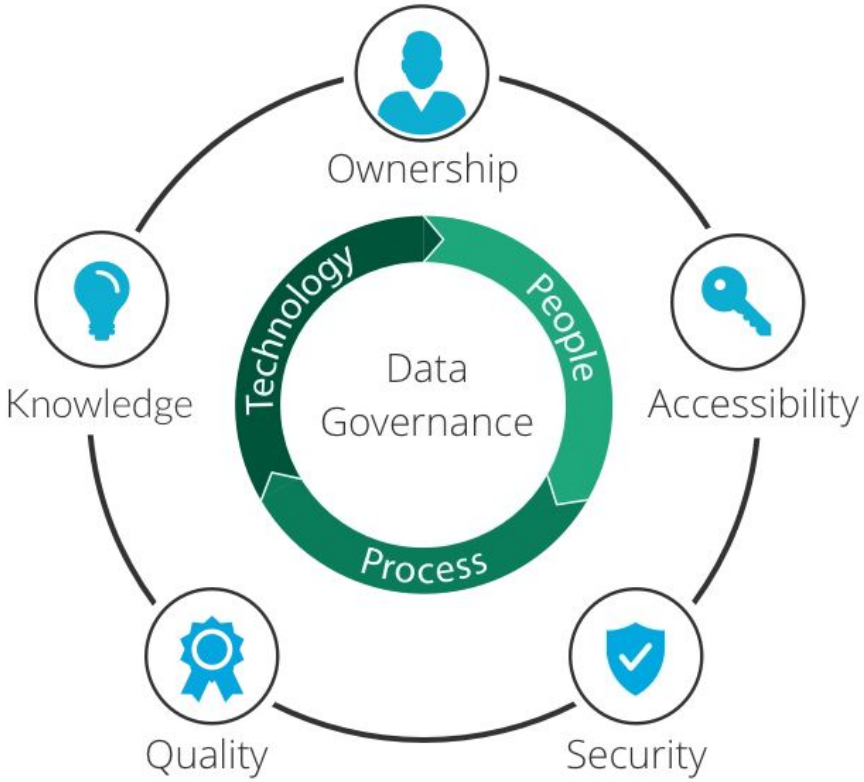


https://www.imperva.com/learn/data-security/data-governance/

Max fine limits for a GDPR infringement as set in 2018: £17.5m or 4% total annual global turnover (whichever is greater)

***Who wants to be the first test case ?***

***https://www.itgovernance.co.uk/dpa-and-gdpr-penalties***

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# Data Management

- No longer just “Where’s my data ?!”
- Securing the data
- Data auditing
- Data classification
- Data encryption
- ***Performance, can we continue to scale ?***
- Resilience
- Data linking
- ***Cost***

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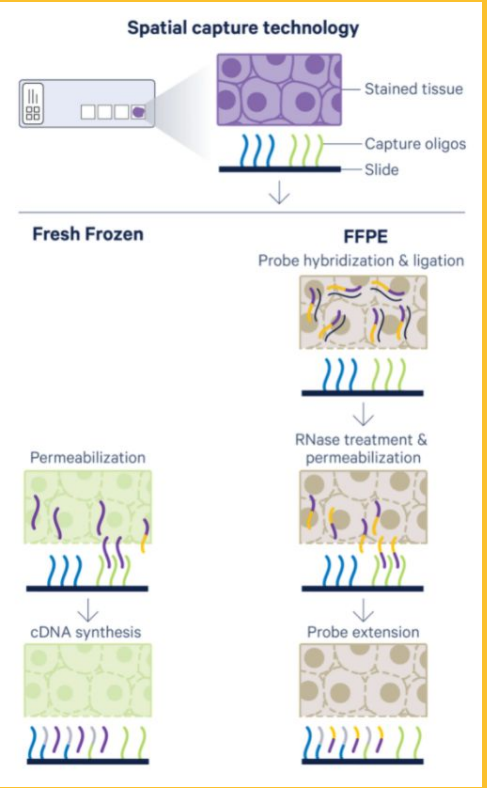
# Oh and our science is growing too

More data-more data-lead science opportunities:

Bring in the microscopes !




https://www.10xgenomics.com/spatial-transcriptomics

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# Linking the data together !

Spatial transcryptomics is potentially a huge area.

No longer “just” sequencing. More data types, greater insights and large scale projects:


https://www.sanger.ac.uk/collaboration/human-cell-atlas/

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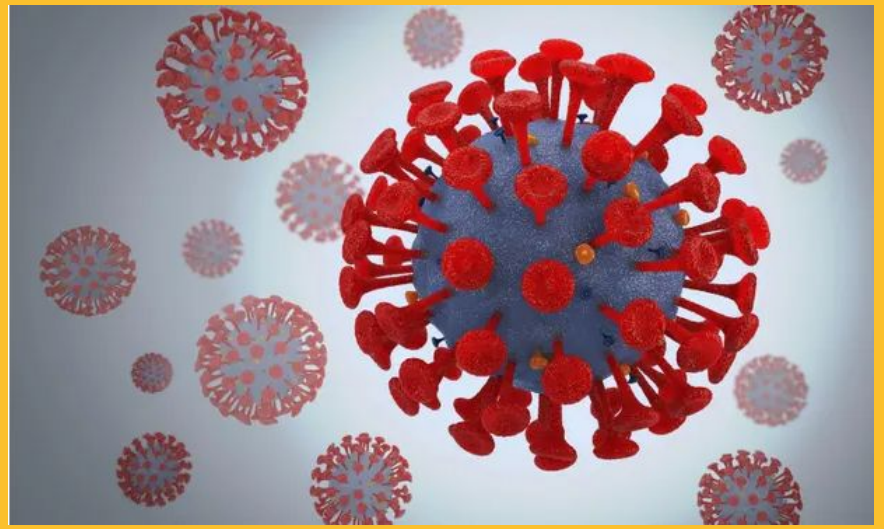
# And then..



https://www.theguardian.com/world/2020/dec/27/scientists-call-for-nationwide-lockdown-after-rapid-spread-of-covid-19-variant

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# Massive call to action.

World wide response to covide has been science lead.

Sequencing and informatics at the center of the fastest ever vaccine development !

https://www.cogconsortium.uk/genomics-in-a-pandemic-shedding-light-on-the-invisible/

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# Project organisation


https://www.cogconsortium.uk/cog-uk/how-we-work/

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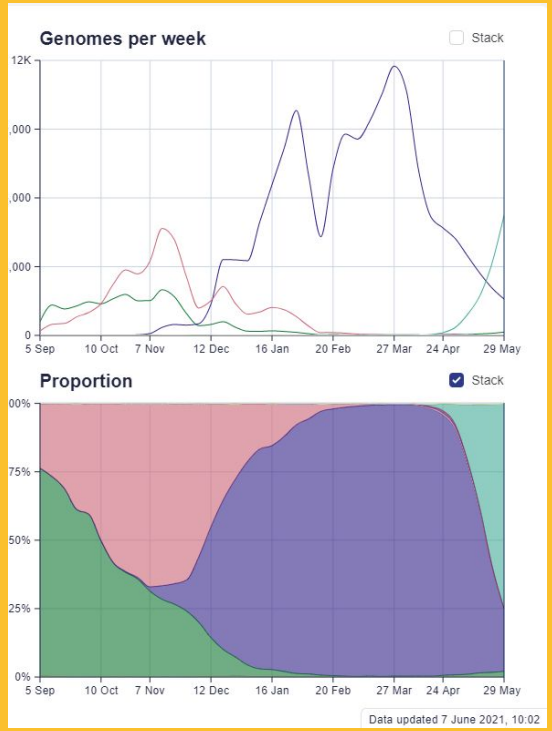
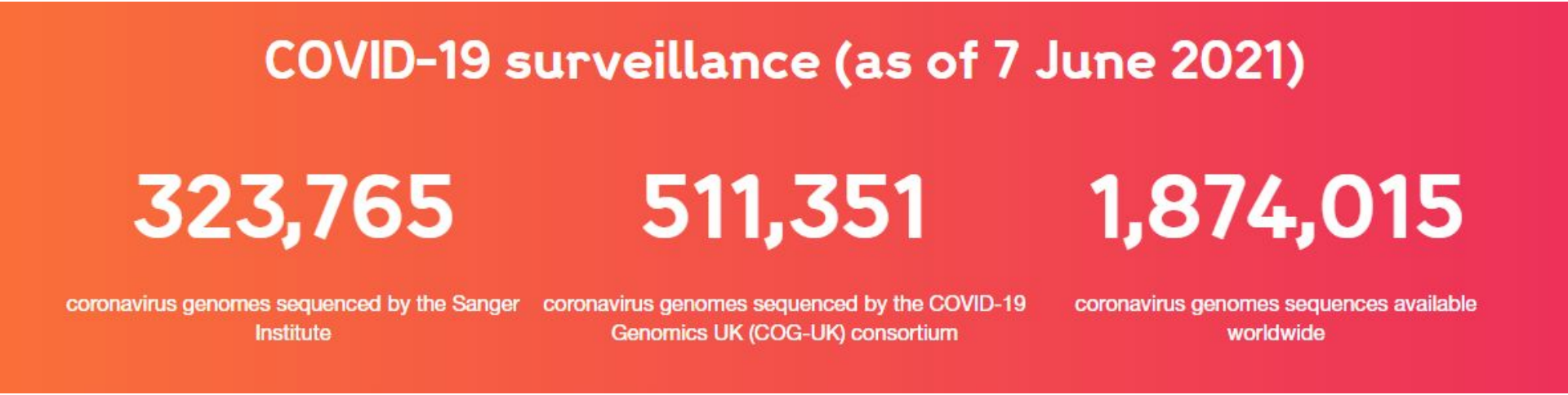
# You can view progress here:




[Lineages (raw) | COVID-19 Genomic Surveillance – Wellcome Sanger Institute]

# Progress to date

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[COVID-19 – Wellcome Sanger Institute]

# So what do we do next ?

Can iRODS alone manage

- The data swell
- Meta-data performance
- Provide 2nd / 3rd gen GUI interfaces
- Provide audit logs and investigative tools
- Simplify customer engagement
- Reduce management churn
- Data security management

Perhaps include some sort of metrics ?

***(managers like metrics)***

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# Is a hybrid solution the answer ?

New data types and services are developing rapidly:

eg:

Genestack

Gen-3

- Would these fill the gap ?
- What would this look like ?
- Will there be best practices for use or is it a DiY suck and see ?
- How would we manage interoperability long term ?
- What does this mean for QA ?
- What does this mean for our teams and developers ?

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# Rays of sunlight

Plugins are coming

For :

- Auditing
- Gen-3
- Indexing
- Improvements to the current GUI

But will they be a part of core ?

***Can we bring new plugins up to speed more rapidly to meet demand while keeping the data-boat afloat ?***

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# So what else have we learned ?

Everything changes.

BUT...

- ***Stay flexible.***
- Stable API's are essential
- Strong auditing and security tools are the future
- Performance is important !
- Reliability, Resilience and Reproducibility are really really important !!
- Remain consistent and avoid surprises !
- ***(sys-admins don't like surprises, unless it's a pay rise !)***
- A trusted partnership is essential !

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# Too many to thank here.

Our original informatics testers !

Thomas Kean

Jim Stalker

NPG

David Jackson and his team past and present !

ISG

See John Constable's presentation later.

Our scientists and informatics teams.

RENCI

Reagon Moore, Leesa ! Terrell, Jason and of course Mike and team !

The community !

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