Chris Dwan - Bioteam

- Scientists with production HPC skills
  - “Bridging the gap between informatics & IT”
  - Vendor & technology agnostic
- A resource for labs and workgroups that don’t have their own supercomputing centers and IT empires
- Various levels of engagement with many clients
  - Gov/EDU/Biotech/Pharma/Fortune-20 clients
  - Work with lots of smart people on common problems
- Tutorial at Edinburgh in 2002 … good to be back.

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Disclaimer

- Most BioTeam clients *don't* have 7 figure IT budgets, Petabyte SANs and dedicated datacenters

- Most of these problems:
  - Simply don't exist for the largest Bio-HPC centers
  - Simply don't matter to the nationally funded Grid projects.

Capital “G” GRID Computing

- Remember the promise?
  - “Utility computing!”
  - “Like turning on a tap!”
  - “Multi-site? No problem!”
  - “Multi-entity? No problem!”
  - “Infinite capacity on demand!”

- GRID Facts in 2008:
  - Still a trainwreck for all but the showcase sites
  - At least the vendor FUD & empty press releases have died down
  - Only a tiny number of showpiece sites have the resources to do “GRID” computing for real

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Observed Trends:

- Clusters: The small cluster market is going away
  - 2-8 node workgroup/lab clusters will be replaced by SMP boxes with multi-core CPUs
- Storage: Same in 2008 as in 2006
  - Unhappy technology tradeoffs
    - The ‘exotic’ vendors offer blazing speed and a few features
    - The ‘mainstream’ vendors exclusively focused on enterprise
    - What I need: Massive scaling, decent speed & grab bag of enterprise features
- Backups:
  - 2006: Backup products not keeping up with daily advances in storage capacity promoted by vendors
  - 2008: On its way to becoming a sick joke

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Observed Trends: Software

- Molecular chemists / CFD folks / single purpose shops know what they want, and how to buy it.
- Despite my best efforts, BLAST is still the state of the art for lots of people.
- Lots of demand in 2007 for single purpose systems designed to run Phylogeny codes
  - PAUP, MrBayes

In-row chilling

1024 Core cluster @ Emory University

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Sealed hot/cold isle enclosures

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Liebert XDO Overhead Cooling

Site: Institute for Computational Biomedicine; Wiell Cornell Medical College

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Next Generation Sequencing

New chemistry: Removes the read length limitation.

10^6 to buy the instrument

Each “run”:

- 5×10^8 base pairs
- 2 - 3 days
- Less than $7,000
- Up to 2TB of raw data

4 vendors, this is 1st revision.

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

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Terrifying: Terabyte Instruments

- Is this your future?
  - Multi-terabyte storage resources in every wet lab?
- Tough decisions ahead
  - Centralized vs. decentralized data capture & movement
- This will effect *everyone* doing HPC “Bio IT”

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The Data Problem

- Primary instrument data (images):
  - ~2TB / day
    - Get used to “peta,” then “exa”.
  - Cheaper to re-sequence than to store?
  - Even if you can store them, TB are still *heavy*
  - Sneakernet lives.

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

- Sequence and quality data:
  - 100 MB / day (manageable)
  - Analysis will have to be local, and accessible to the lab scientists.
  - What will NCBI do?

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Next-gen Sequencing

- Vendors want lock-in, scientists do not
- Initial data processing may keep up, re-processing will not
  - C.f: Microarrays
- This is the *first* generation. Core assumptions are still fluid.
- Opens the HPC market to a whole bunch of new users (physicians, security, environmental monitoring, …)

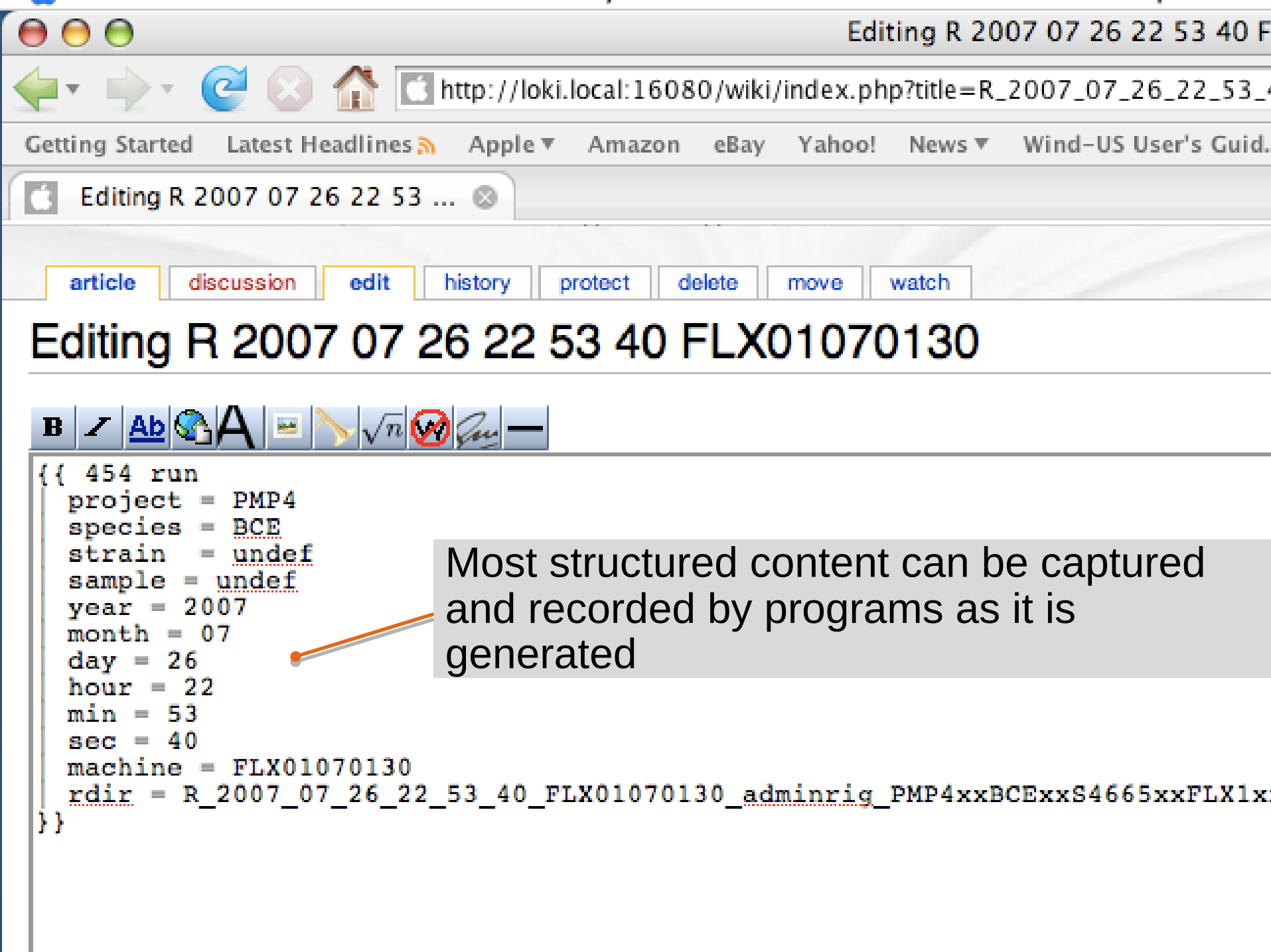
Wikilims: Next Gen Data Store

Meta data

wiki

File data

raid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http://loki.local:16080/wiki/index.php?title=R_2007_07_26_22_53_
Getting Started
Latest Headlines
Apple
Amazon
eBay
Yahoo!
News
Wind-US User's Guid.
Editing R 2007 07 26 22 53 ...
article
discussion
edit
history
protect
delete
move
watch
Editing R 2007 07 26 22 53 40 FLX01070130
{{ 454 run
project = PMP4
species = BCE
strain = undef
sample = undef
year = 2007
month = 07
day = 26
hour = 22
min = 53
sec = 40
machine = FLX01070130
rdir = R_2007_07_26_22_53_40_FLX01070130_adminrig_PMP4xxBCExxS4665xxFLX1x
}}
Most structured content can be captured and recorded by programs as it is generated

Parent: Species YFR
Siblings: Other YFR strains
Children: NS2456 cultures

Update NS2456 dashboard

NS2456 updated Fri Oct 19 03:48:49 2007	
R_2005_02_15_13_03_34_rig13_mbenitez_2577426060012805C20G4R4 reanalyze	D_2007_10_04_15_02_42_runImagePipe D_2006_10_04_18_23_12_runImagePipe D_2005_09_01_16_24_56_runImagePipe
R_2005_02_10_11_30_13_rig9_baltman_2577606042012805C20G4r3 reanalyze	D_2007_10_05_10_59_24_runImagePipe D_2006_10_04_12_18_13_runImagePipe D_2005_09_01_14_31_11_runImagePipe
R_2005_02_08_12_58_29_rig11_baltman_2577606042012805C20G4r2 reanalyze	D_2007_10_09_08_59_48_runImagePipe D_2006_10_04_06_51_28_runImagePipe D_2005_09_01_12_37_00_runImagePipe
R_2005_02_03_10_16_21_rig13_baltman_2577606042011205C20G4r1 reanalyze	D_2007_10_09_17_47_21_runImagePipe D_2006_10_04_01_24_12_runImagePipe D_2005_09_01_10_50_52_runImagePipe

assemble

Launch an assembly on the cluster

P_2007_10_20_04_34_08_loki
P_2007_10_20_04_34_44_loki
P_2007_10_20_04_38_43_loki

resources
- iNquiry Portal
- WikiLIMS
- LabCollector
- MySQL-Admin
- GBrowse

development
- SVN
- CVS
- TRAC

search
Go Search

toolbox
- What links here
- Related changes
- Upload file
- Special pages
- Printable version
- Permanent link

Potential trend: Data Triage

- In 2007 first decisions to not store primary data
- In the past
  - Always keep *all* data, essentially forever
  - Excuses:
    - It costs to much to repeat the experiment
    - Experiment can't be repeated (imaging, microscopy)
    - *"It's just too horrible to think about"*
- Moving forward (2008 and beyond)
  - Expect cost/benefit discussions among IT and scientific staff
  - What data *really* needs to be kept? (Primary vs. Derived data)
  - In what cases is it actually be cheaper to rerun the experiment?
  - MAID - Massive Array of Idle Disks

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Amazon EC2 for Bio Apps

- Thanks Dr. Papadopoulos!
- BioTeam *is*:
  - Enthusiastic about Amazon EC2 & S3
  - Considering building EC2-aware products
    - Desktop, cluster & standalone GUIs
- BioTeam *has*:
    - MPIBLAST running on EC2
    - MrBayes-MPI running on EC2
    - Cross platform GUIs for both applications
    - Generic Sun Grid Engine EC2 images (*in development*)
  - Storage for both coming from within Amazon S3
  - Many more apps on the way …

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Amazon EC2 for Bio Apps

- Why EC2?
  - The economics are compelling
    - One month of serious experimentation:
      - $9.00 USD billed to credit card
  - Various money making approaches
    - Flexible pricing allows reselling & revenue sharing
    - I can create a EC2 image and add my own fees on top to cover development and support costs
  - I don’t need your credit card
    - Amazon handles all transactions & billing

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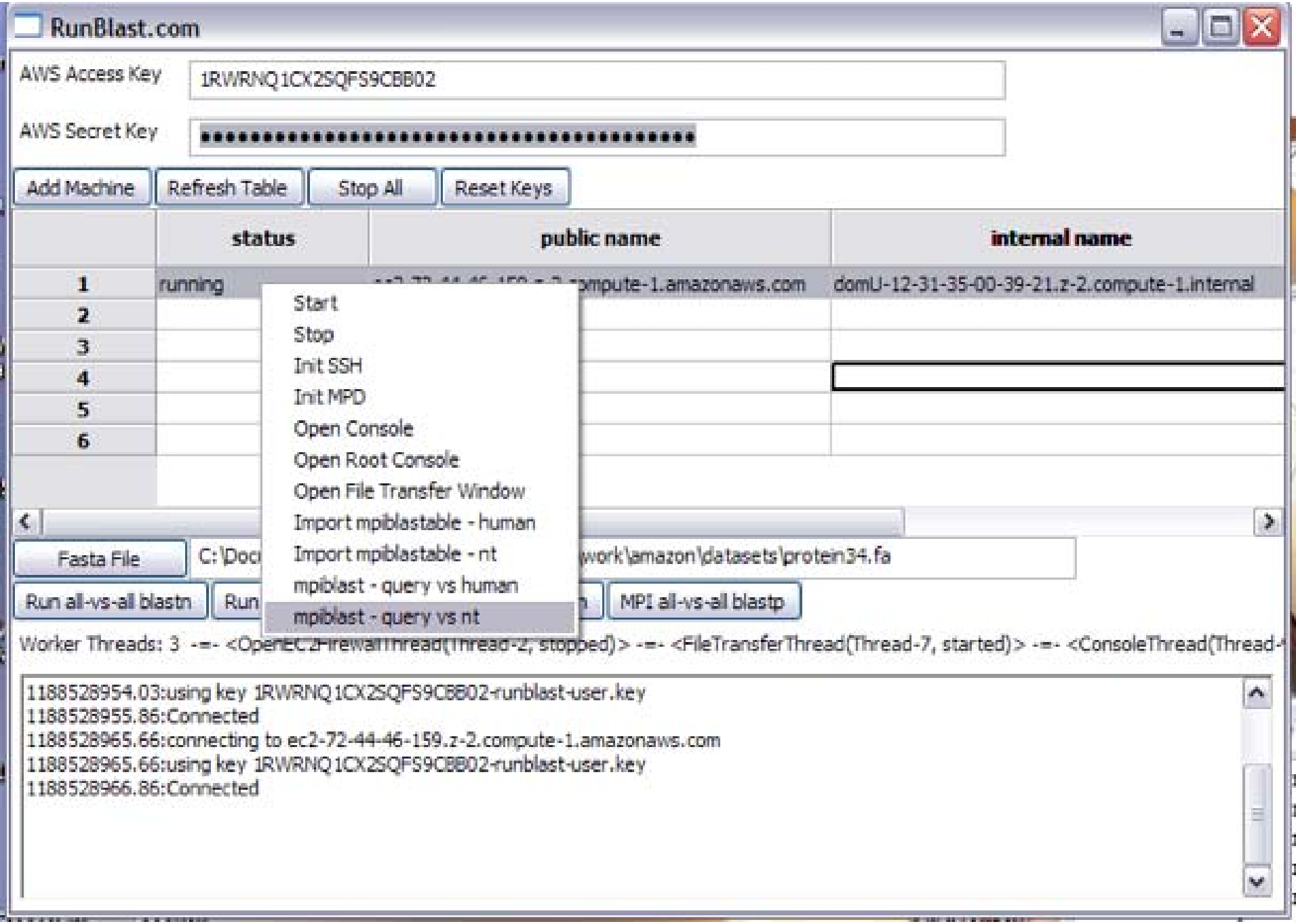

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Conclusions

- Data is the problem
  - Storage and Backups are not keeping pace with requirements
  - This is forcing scientists to revisit core assumptions
- CPUs are not as big a problem
  - Clusters are commodity
  - Cloud augments one-off needs.
- Smaller labs are rolling their own solutions
- As usual, the biggest problems are social / political.

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