Welcome to AG Retreat IV

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The Vision

- In 1994 I asked the question
  - What if travel was instantaneous and free?
  - How would this change your world ?
- The AG is the closest thing we have to making this a reality
  - It is starting to change the world
- But we can do better!!

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Our Challenge

- Create a high-quality development platform for a new class of applications
  - Human oriented
  - Tools that are easily integrated with Grids
  - Multiple OS and HW targets (Windows, Linux, Mac)
- Encourage spontaneous deployment
  - Empower groups in academia, government and industry
  - Address the mobility issues important to our generation
- Focus on the future
  - Upscale the capabilities (HDTV, HD audio, tiled displays)
  - Gigabit/sec Access Grid is around the corner

The Big Picture Goals

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- Safe and abundant food supplies
- Sustainable and benign energy sources
- Effective management of disease and aging
- Novel materials and renewable industrial feedstocks
- Advanced computational devices beyond Moore's law
- Wide variety of molecular scale machinery
- Self-assembly and self-reproduction technologies

Targets for Advanced AG Capability

- Fusion Collaboratory (DOE)
- Advanced Photon Source Collaborative Access Teams (DOE, NSF)
- Cancer Bioinformatics Grid (NIH)
- National Microbial Pathogen Data Center (NIH)
- Center for Learning and Multimodal Communication (NSF)
- Advanced Biomedical Consortium (NIH)
- International Systems Biology Grid (DOE, NSF, NIH, EU)
- Deployable Field Stations (NSF, DOE, others)
  - Microbial Ecology
  - Environmental Imaging
  - Archeology and Paleontology

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Where are We Heading

- Integration of instruments and imaging devices
  - Sensors, scanners, microscopes, and rangefinders etc
- Integration of advanced visualization capabilities
  - Stereo, very high resolution and immersive displays etc
- Improved video and audio capabilities
  - HD video, multi-channel studio quality audio
- Rich suite of groupware plug-ins
  - To do lists, workflows, voting tools, agenda tools, etc.
- Collection of innovative collaborative applications
  - Steering and visualization, web tools, portals,

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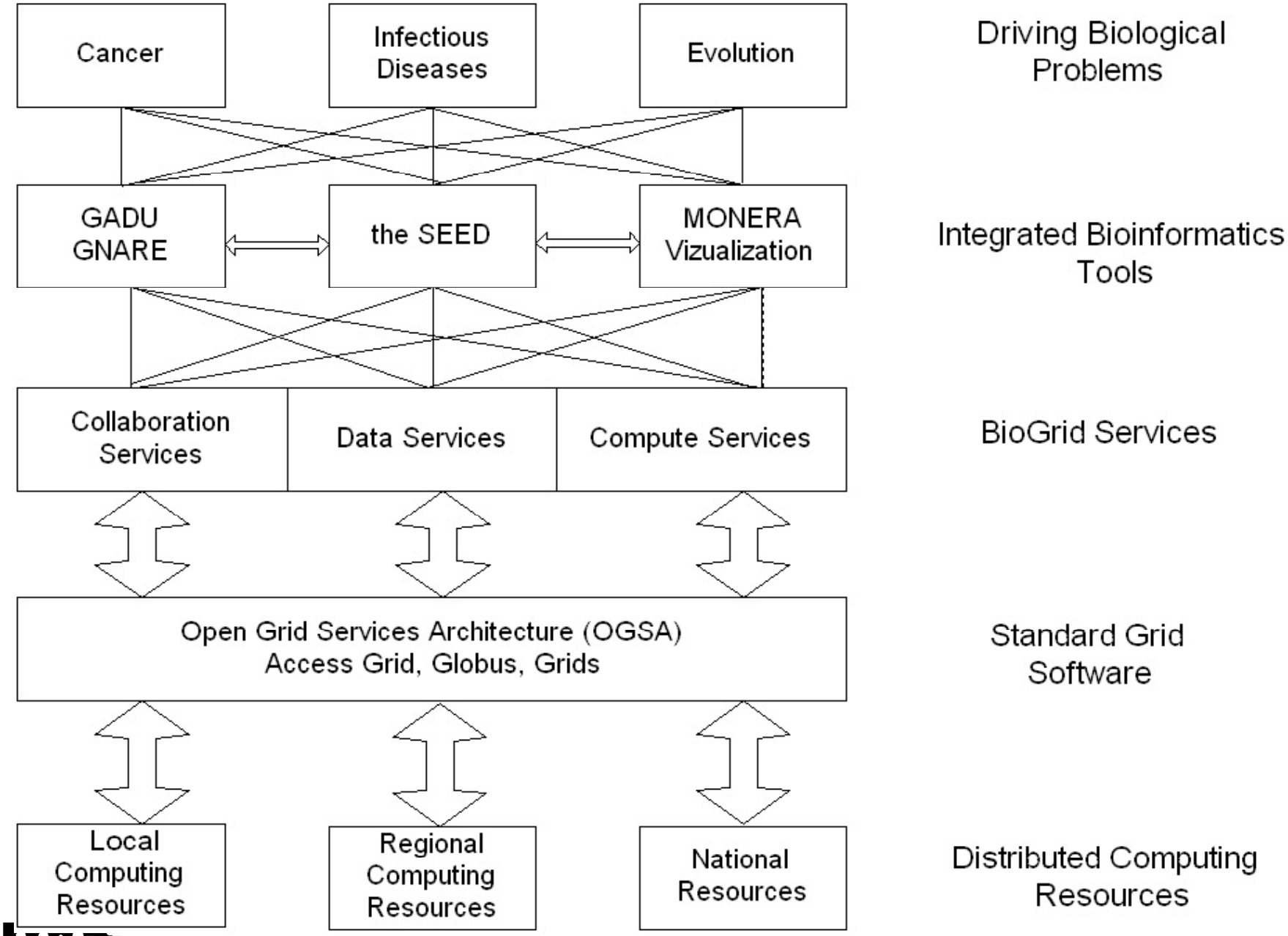
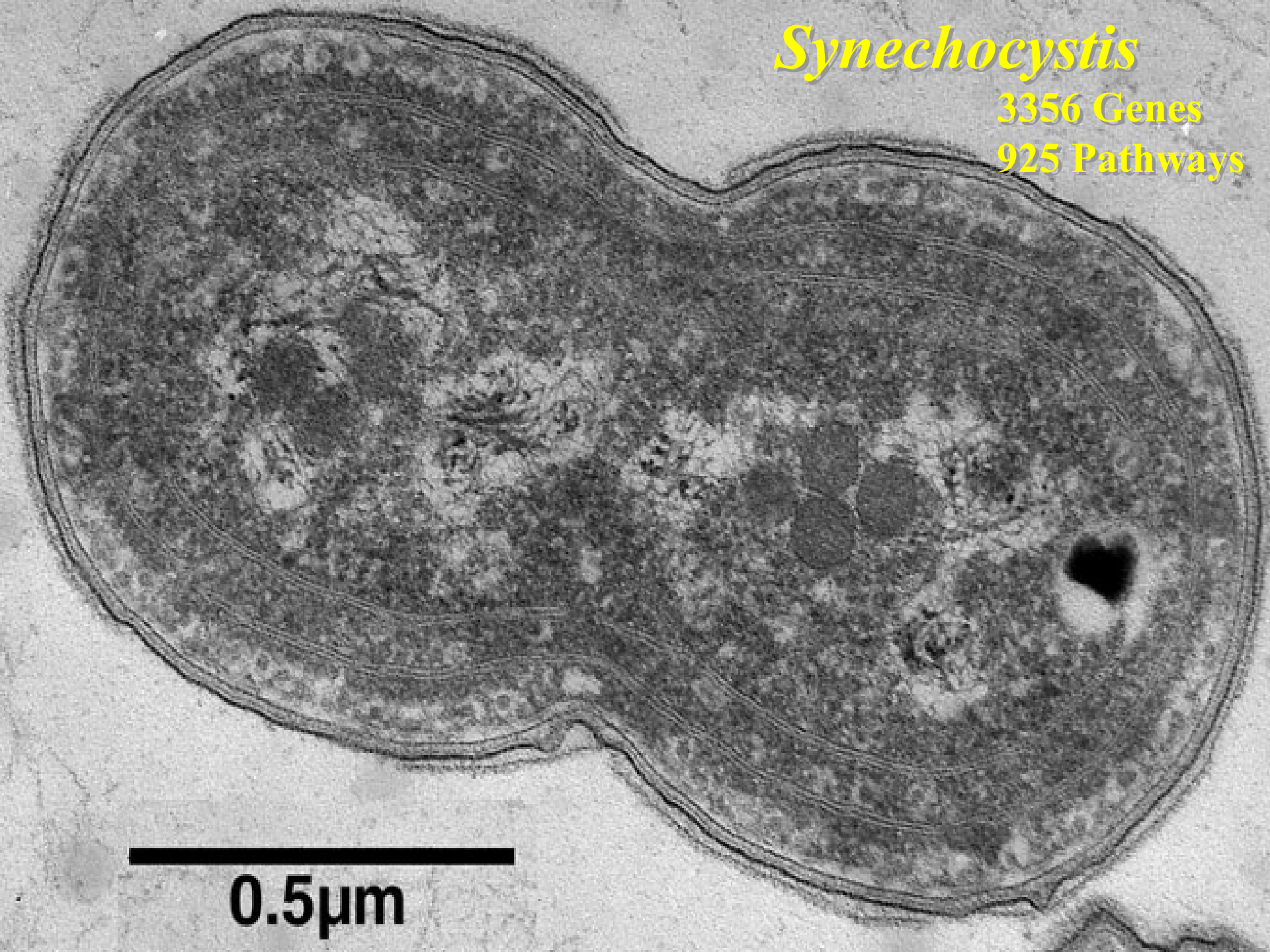
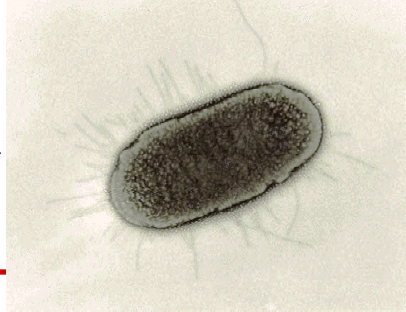
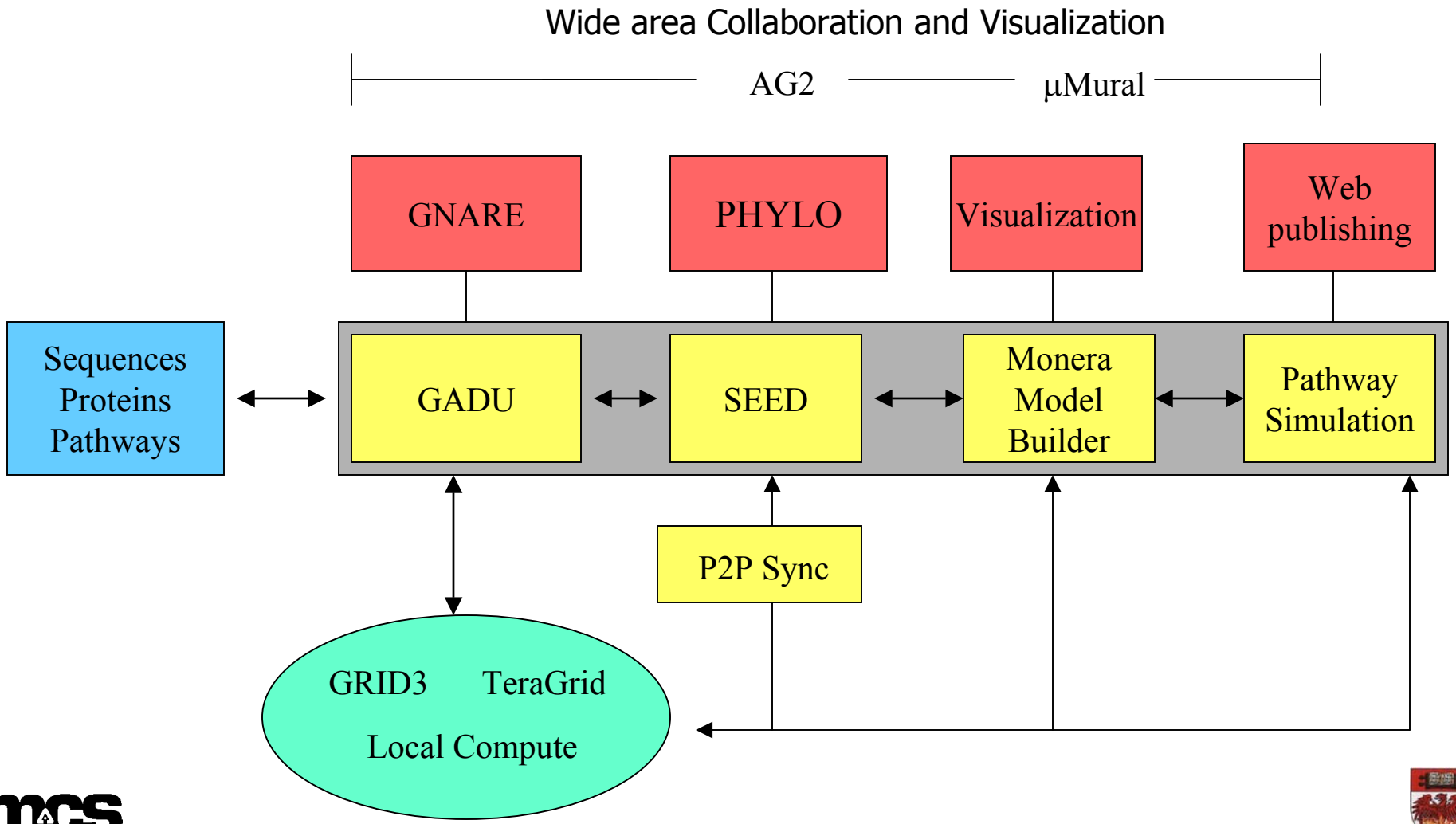
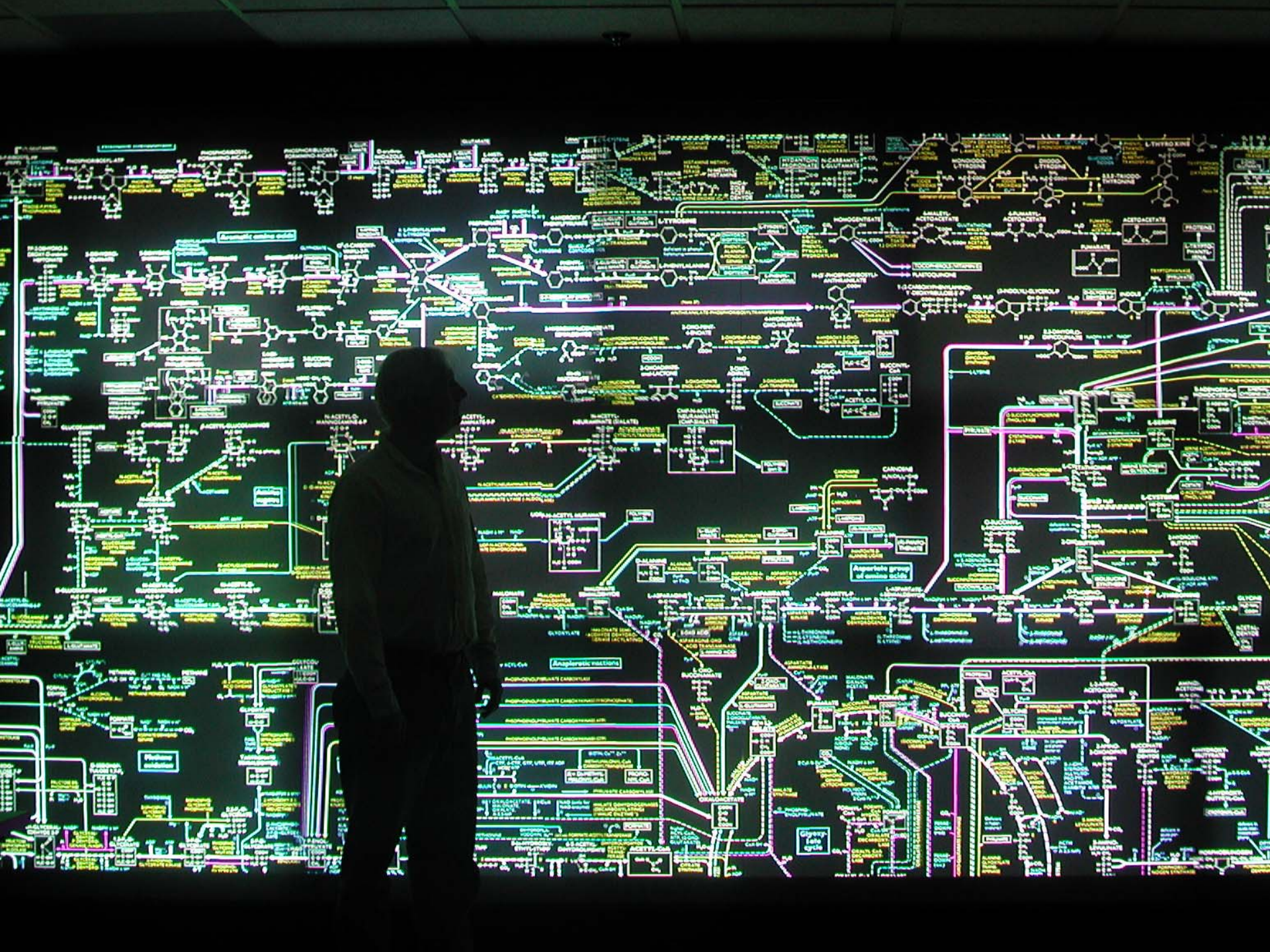

Cancer
Infectious Diseases
Evolution
Driving Biological Problems
GADU GNARE
the SEED
MONERA Vizualization
Integrated Bioinformatics Tools
Collaboration Services
Data Services
Compute Services
BioGrid Services
Open Grid Services Architecture (OGSA)
Access Grid, Globus, Grids
Standard Grid Software
Local Computing Resources
Regional Computing Resources
National Resources
Distributed Computing Resources


Synechocystis
3356 Genes
925 Pathways
0.5µm

Argonne Systems Biology Workflow







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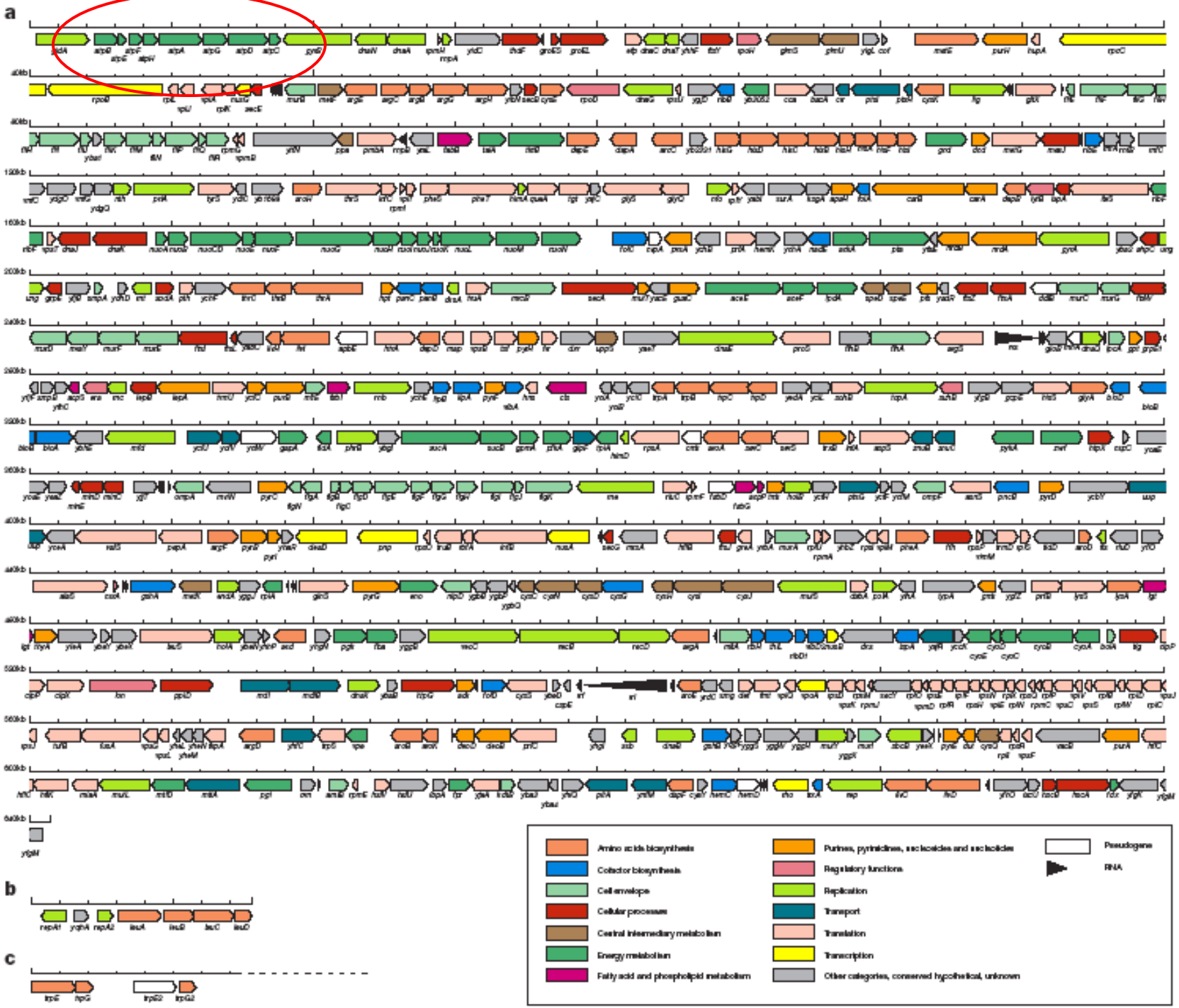
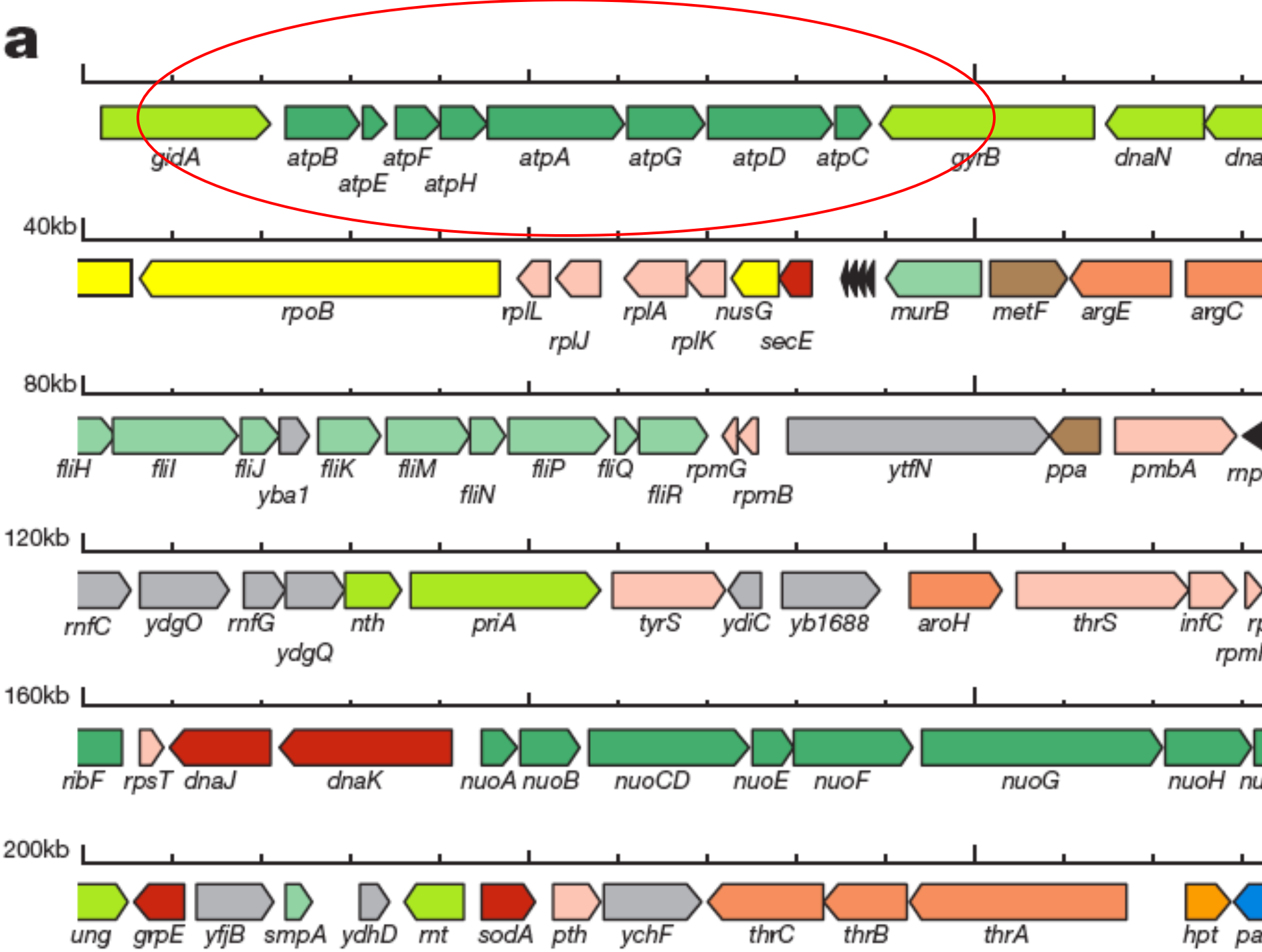
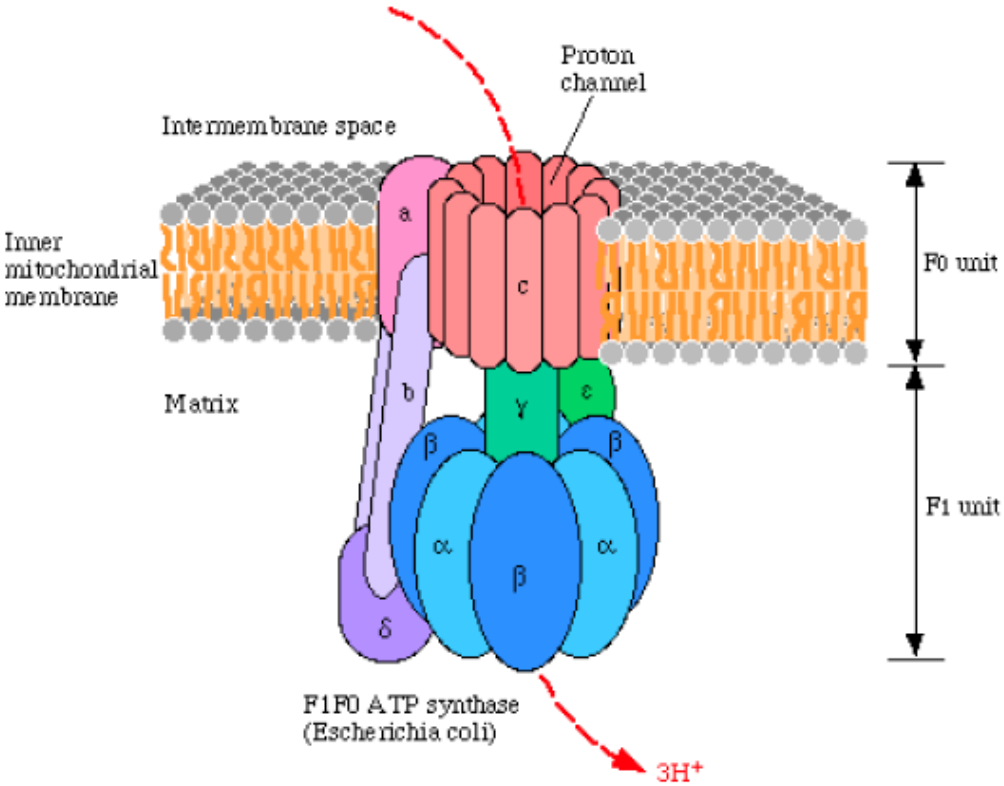

a
b
c
Amino acids biosynthesis
Cofactor biosynthesis
Cell envelope
Cellular processes
Central intermediary metabolism
Energy metabolism
Fatty acid and phospholipid metabolism
Purines, pyrimidines, nucleosides and nucleotides
Regulatory functions
Replication
Transport
Translation
Transcription
Other categories, conserved hypothetical, unknown
Pseudogene
RNA


a
gidA
atpB
atpE
atpF
atpH
atpA
atpG
atpD
atpC
gyrB
dnaN
40kb
rpoB
rplL
rplJ
rplA
rplK
nusG
secE
murB
metF
argE
argC
80kb
fliH
fliI
fliJ
yba1
fliK
fliM
fliN
fliP
fliQ
fliR
rpmG
rpmB
ytfN
ppa
pmbA
120kb
rnfC
ydgO
rnfG
ydgQ
nth
priA
tyrS
ydiC
yb1688
aroH
thrS
infC
160kb
ribF
rpsT
dnaJ
dnaK
nuoA
nuoB
nuoCD
nuoE
nuoF
nuoG
nuoH
200kb
ung
grpE
yfjB
smpA
ydhD
rnt
sodA
pth
ychF
thrC
thrB
thrA
hpt

ATP SYNTHESIS



F-type ATPase (Bacteria)

beta	alpha	gamma	delta	epsilon	c	a	b

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Multiple Sequence Alignments

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Large-Scale Computing and the Hunt for Horizontal Gene Transfer

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- Organismal Trees
  - 16S rRNA subunit
  - Trees from multiple genes (e.g. Ribosome proteins)
- Gene Trees
  - Phylogeny for ~1000 most conserved genes x ~200 organisms
  - Core metabolism (TCA, EMP, PPP), DNA replication and repair, nucleotide synthesis, amino acid biosynthesis, etc.
- Operon Trees
  - Phylogeny for ~50-100 more conserved operons (gene clusters)
- Reconciliation
  - Sorting events, co-speciation, duplication, horizontal transfer
  - About 1 million reconciled trees will be generated

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Welcome

- Thanks to everyone involved in making this retreat possible
- Everyone here can play an important role in making the AG a success
- The AG community has accomplished a lot in the last five years, but much remains to be done
- Breathe Deep and Fly High!!

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