Texas A&M

Supercomputing Facility

Boosting Productivity with Advanced User Services

Raffaele Montuoro

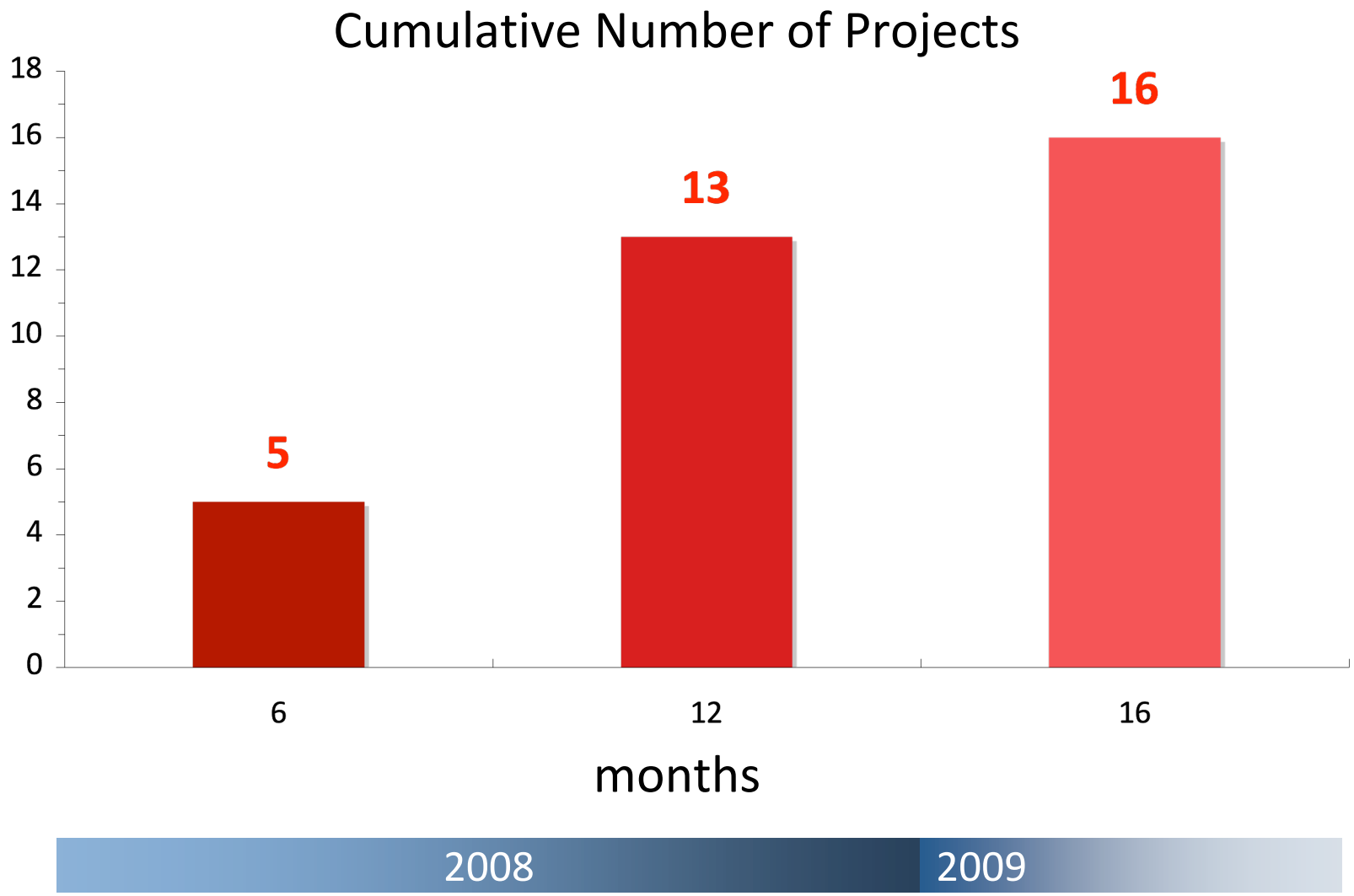
Advanced User Services: Mission

- Enhance and support computational sciences within Texas A&M University

Advanced User Services: Details

- Performance Analysis of computer codes
- Code Optimization
- Code Parallelization: OpenMP & MPI
- Consulting for code development on SC systems
- Code Porting on the SC systems
- Tune up of common scientific applications
- Benchmarking
- Design and configuration of small computer clusters

Advanced User Services: Young, but Tall



Advanced User Services: A Closer Look

- SODA: A Simple Ocean Data Assimilation Model

  Dr. Benjamin Giese, Dept. of Oceanography

- MST: Material Simulation Tool

  Dr. Tahir Cagin, Dept. of Chemical Engineering

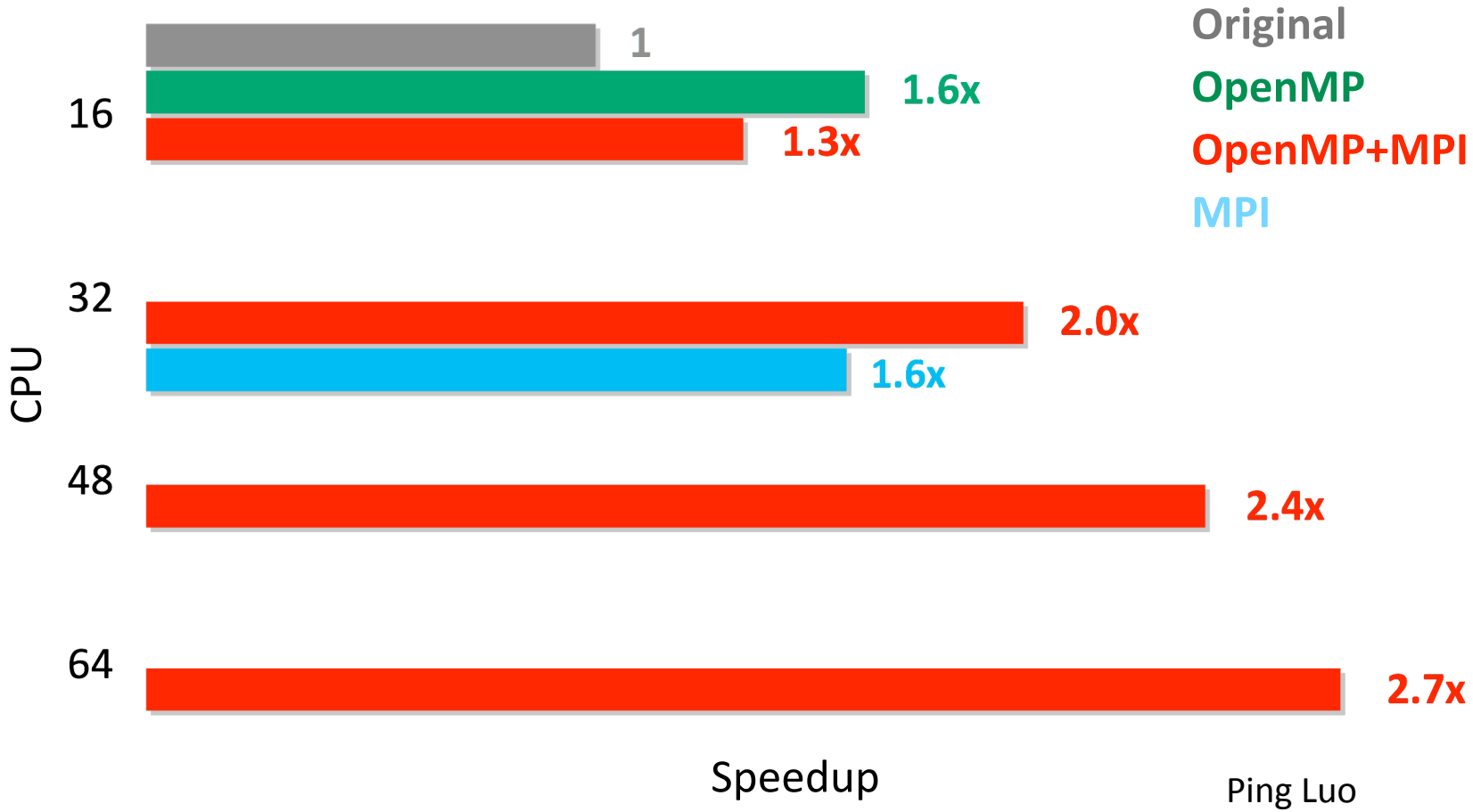
- Illumina Genome Analysis Pipeline

  Dr. James Sacchettini, Dept. of Biochemistry and Biophysics

SODA: Simple Ocean Data Assimilation

B. Giese

Original Code: FORTRAN/OpenMP Case: 2004-01-20



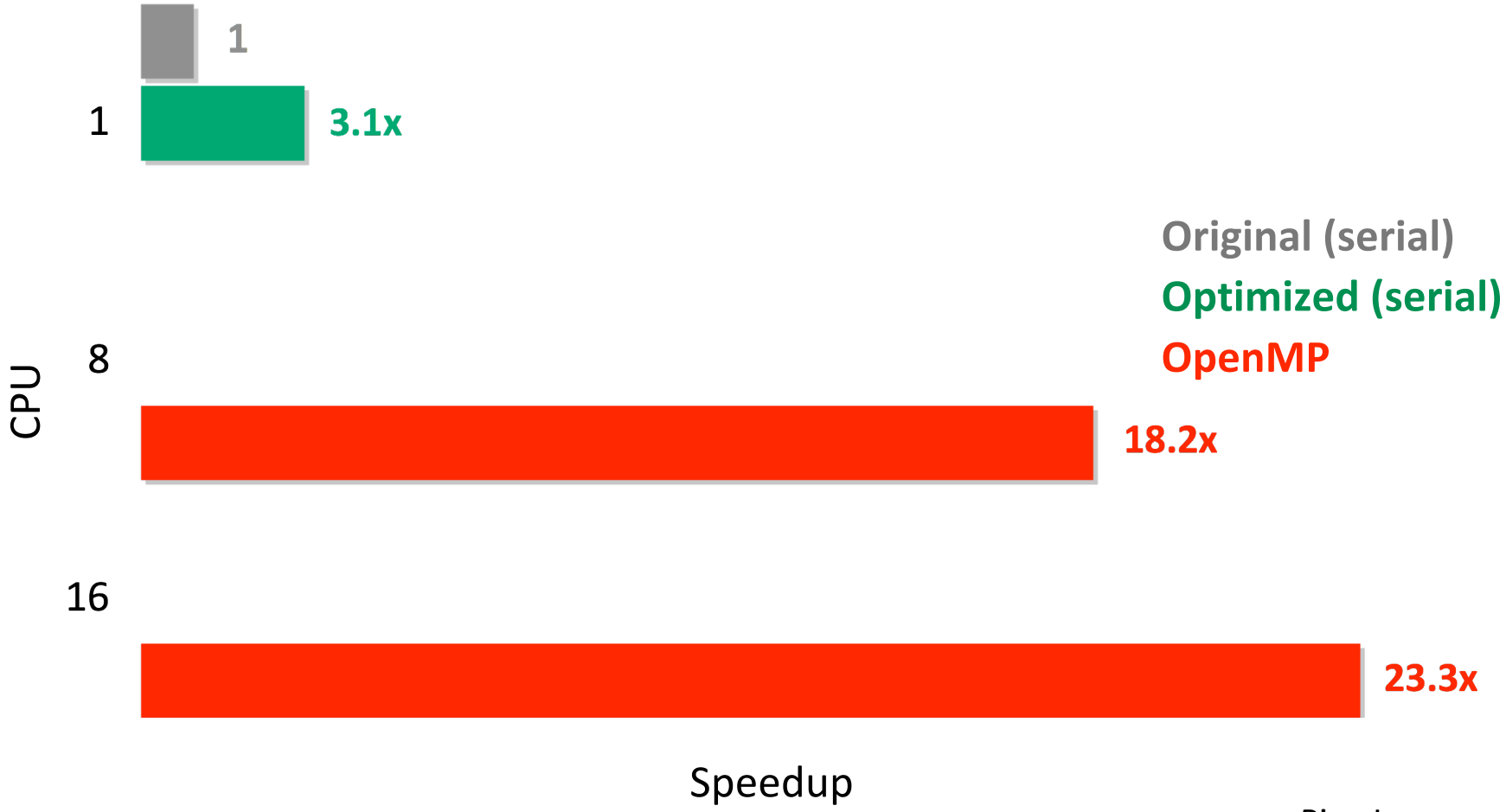
Ping Luo
Xiandong Meng
SC staff

Material Simulation Tool

T. Cagin

Original Code: C++, serial

Case: 101010



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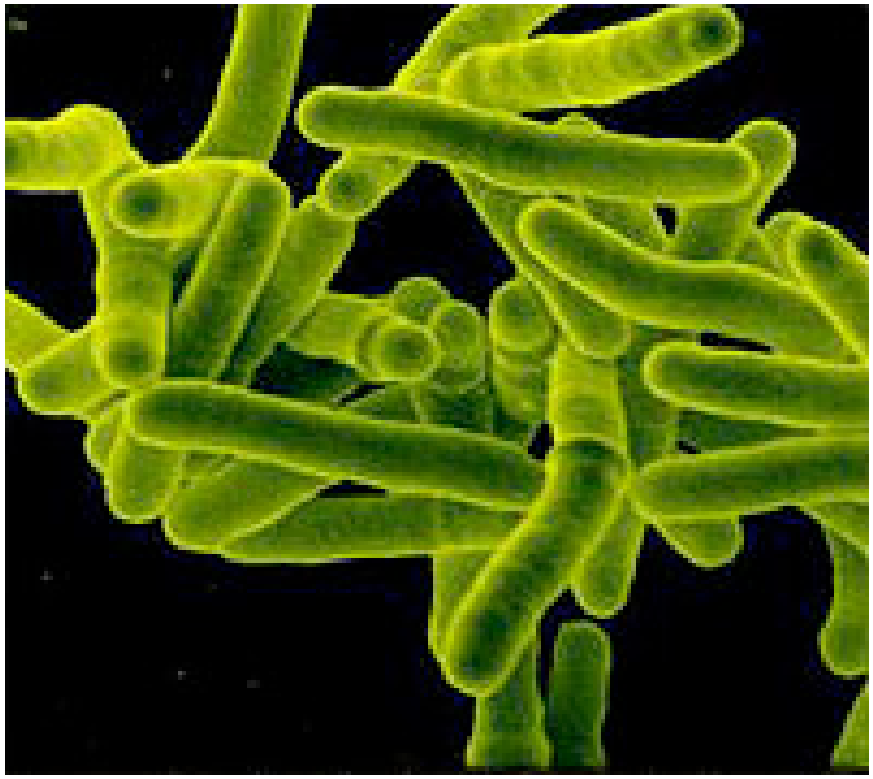
SC staff

Parallel Genome Analysis Pipeline

J. Sacchettini
T. Ioerger

Bio- and Chemi- Informatics:
Studies on *M. tuberculosis* Drug Action & Resistance



Whole genome sequencing can be used to define the mechanism of drug action and resistance.

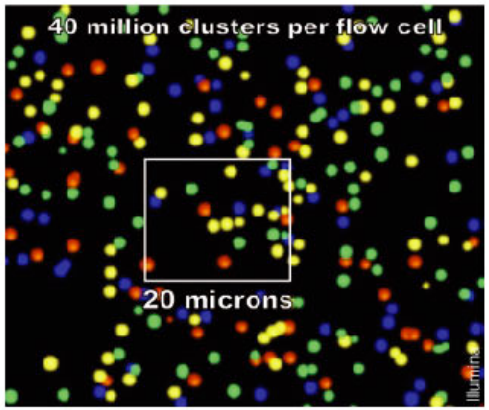
Parallel Genome Analysis Pipeline

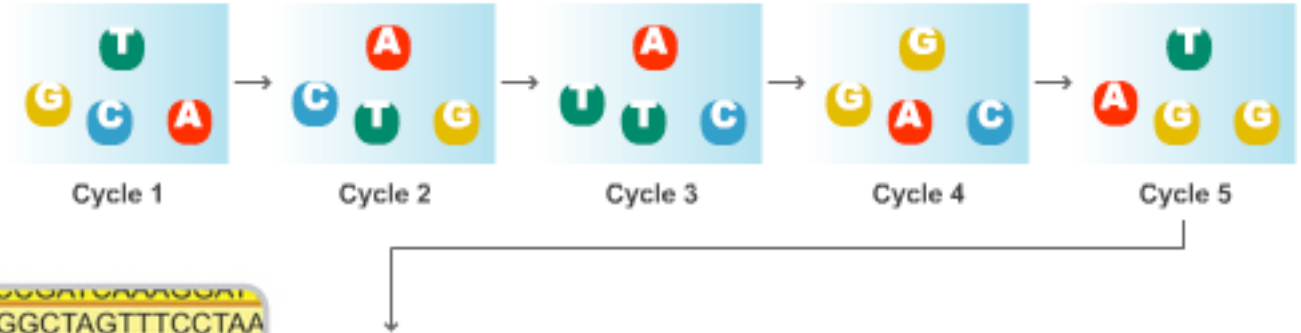
J. Sacchettini
T. Ioerger

How Solexa sequencing works

Single-ended sequencing:

1) Fragment gDNA select 200-300 base fragments
2) Spread and attach fragments to a lane on a chip, amplify
3) Press go





4) Just align your short reads, allowing gaps/mismatches, against a reference genome, and look for snps and indels

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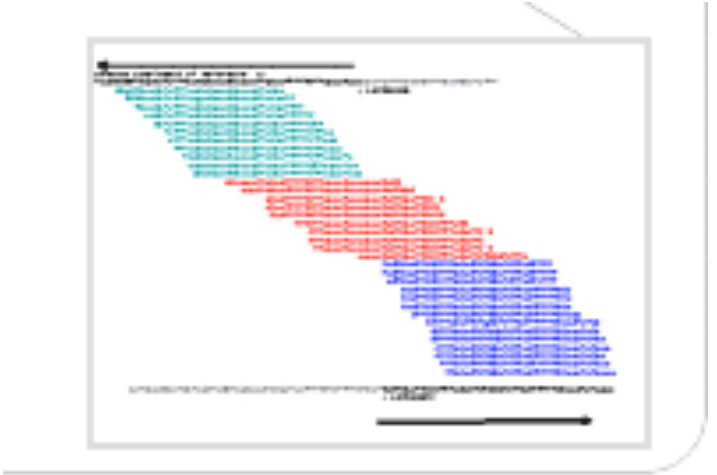
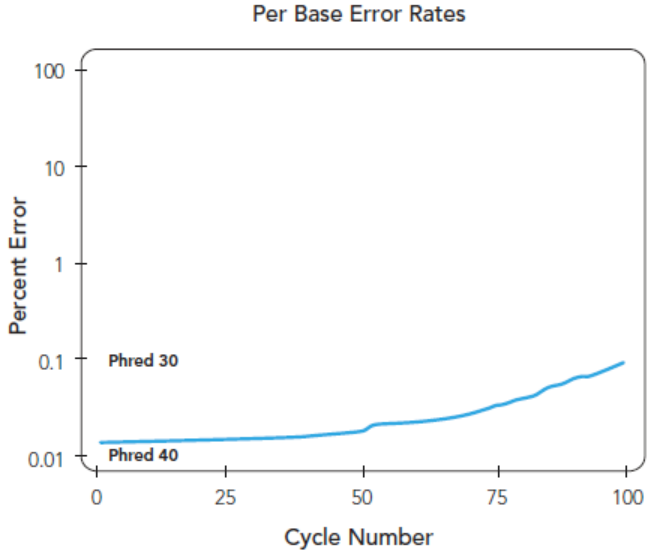
What can you do with all that sequence?

Sequence an entire genome of Mtb
—4M bases in the Mtb genome

Therefore with 20Mx36 base reads you get 100% coverage with 200-fold redundancy- (depth of coverage) per genome; 7 genomes per chip

Or you can add a tag to each of 4 genomes and run them on a single lane -50 fold depth of cover per genome- 28 genomes per chip





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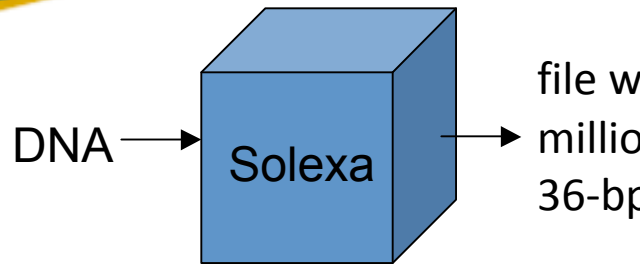


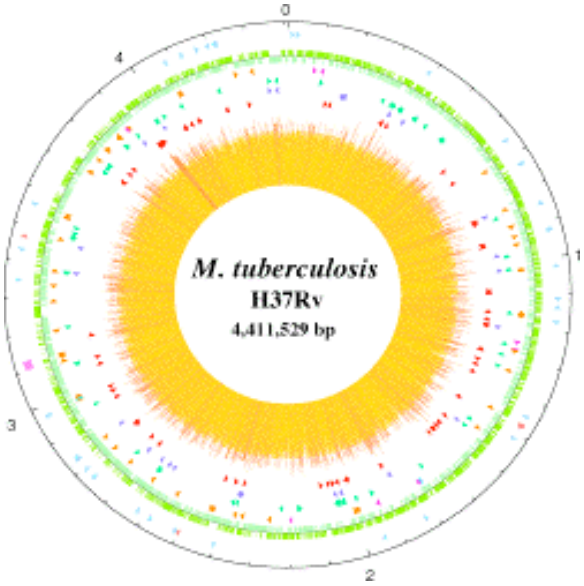
file with millions of 36-bp reads

align reads against reference genome

identify *putative SNPs* where majority base differs from expected base

build *local contigs* in surrounding ~200 bp and align against reference genome to identify true SNPs vs. indels

edit genome sequence and realign reads



Ioerger Sequencing Protocol

Parallel Genome Analysis Pipeline

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- Solexa's Genome Analysis Pipeline is a customizable analysis engine capable of taking the raw image data generated by the Genome Analyzer and producing intensity scores, base calls, and quality metrics, and quality scored alignments
- Based on Makefile
- Scales up to 8 shared-memory tasks (`gmake -j 8`)
- Typical problem size: 8 lanes x 36 cycles x 4 bases x 100 images/base/cycle = **115,200** images to be processed

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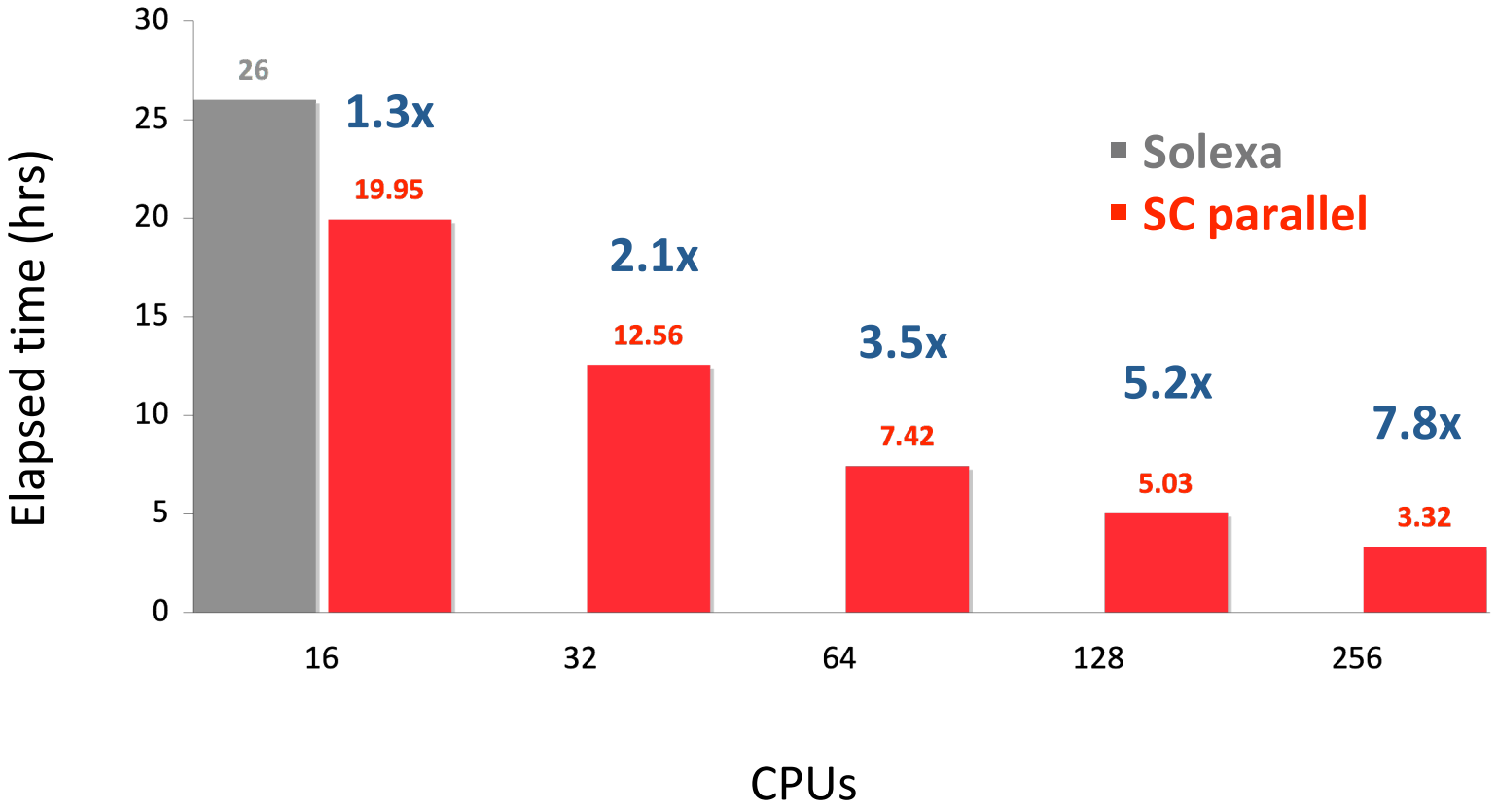
ANALYSIS none, 79 cycles, **252,800** images



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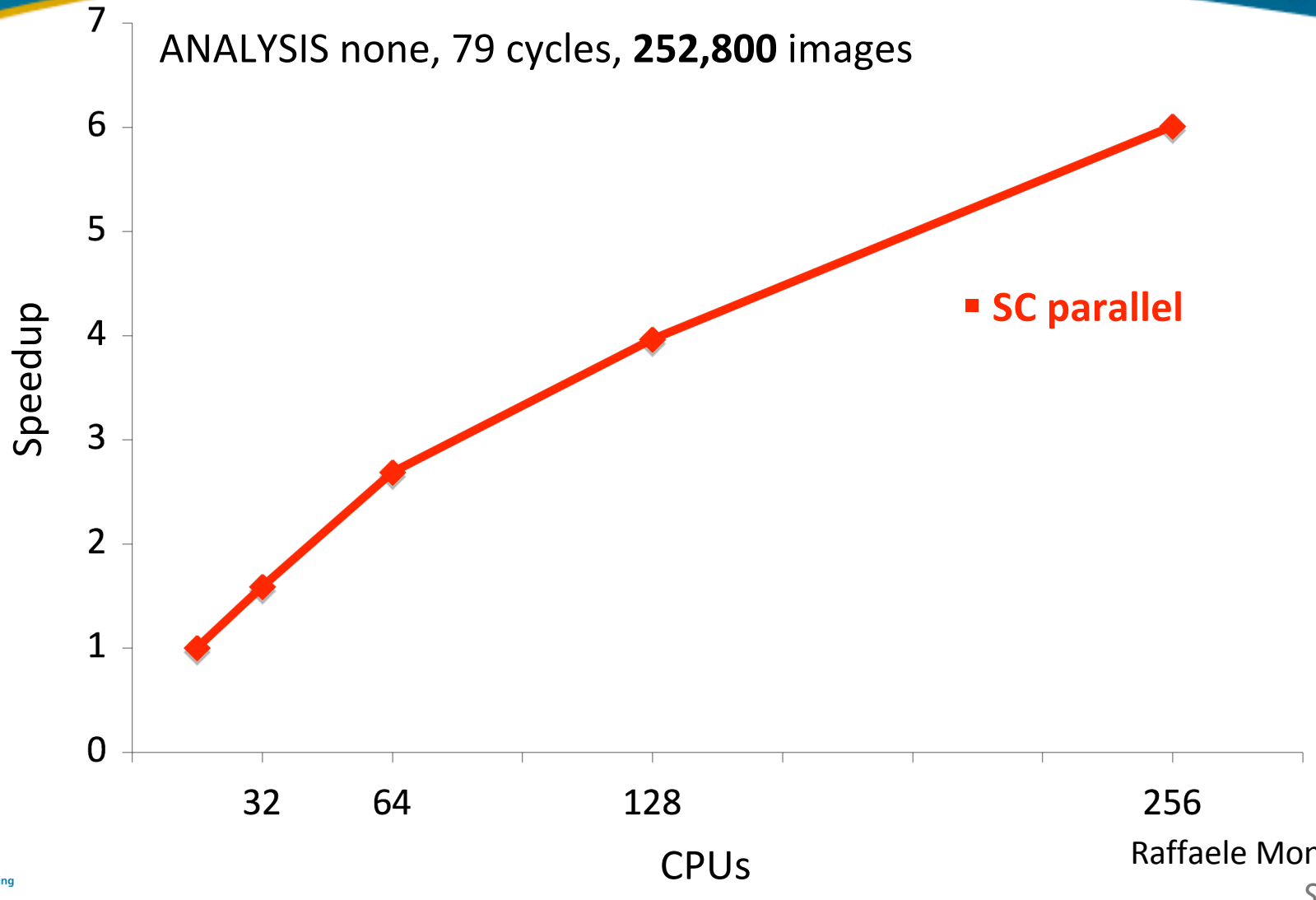

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Advanced User Services

Q: How to apply?

A: E-mail the Supercomputing Help Desk:

help@sc.tamu.edu