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Microbiological and Geological Systems

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CAMS Planning Workshop
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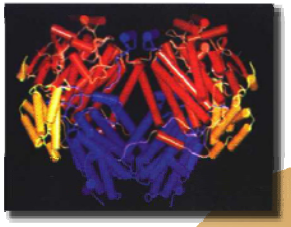
Complexity

Unique capabilities such as the geocentrifuge allow us to accomplish temporal scaling

Vision: By 2015 INL will lead the science to understand, predict, and control microbial metabolic systems in complex geologic environments.

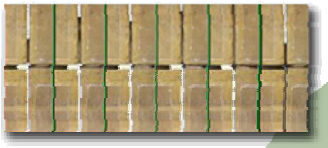
Metabolic pathway models are at the forefront of predictive biology



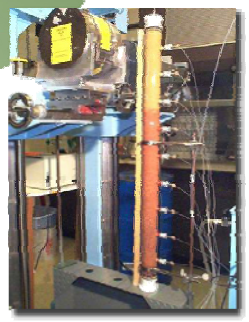
System Behavior

Modeling

Physical processes such as pore scale fluid flow will be linked to microbial metabolic activity



Microbial communities within complex environments possess diverse capabilities

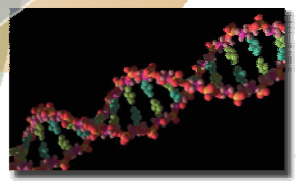


Intermediate scale column experiments bridge the gap between molecular scale processes and field scale observations

Scale

Systems Microbiology

Experimental Geoscience



DNA provides the blueprint for microbial function

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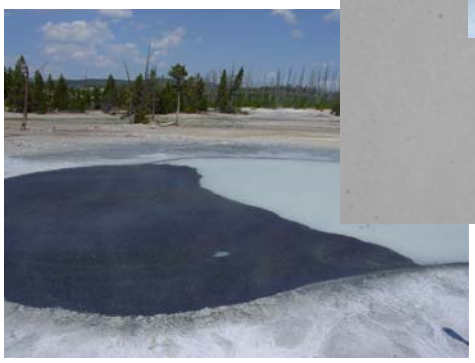

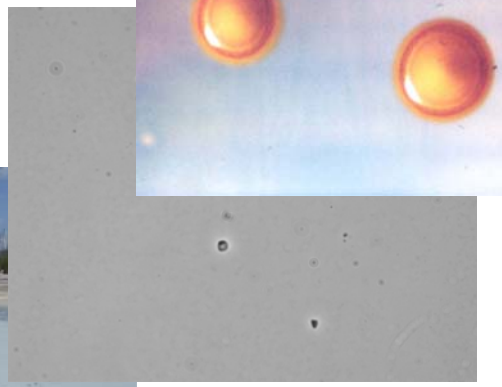

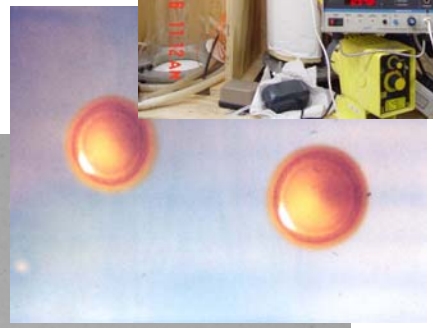

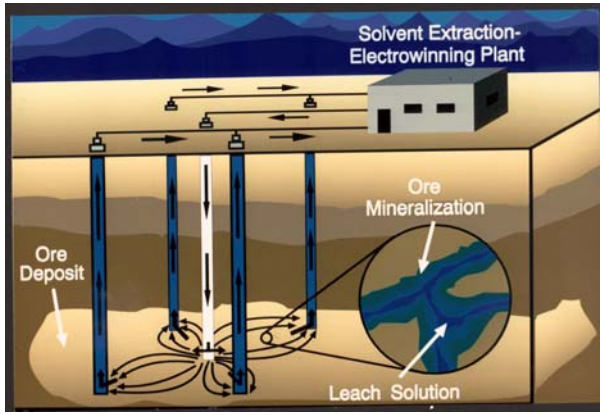

Biomining – a real world challenge for the bio-geo signature

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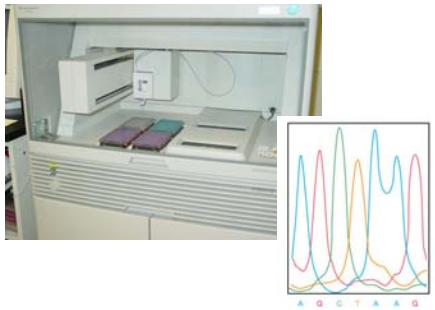
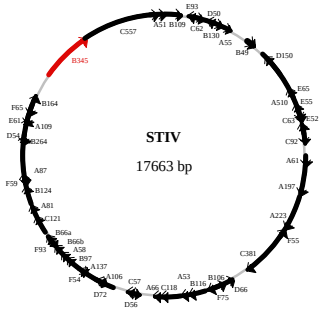
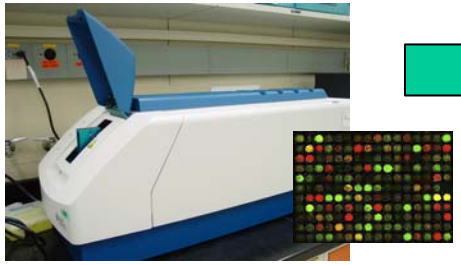
The INL Bioinformatics Pipeline



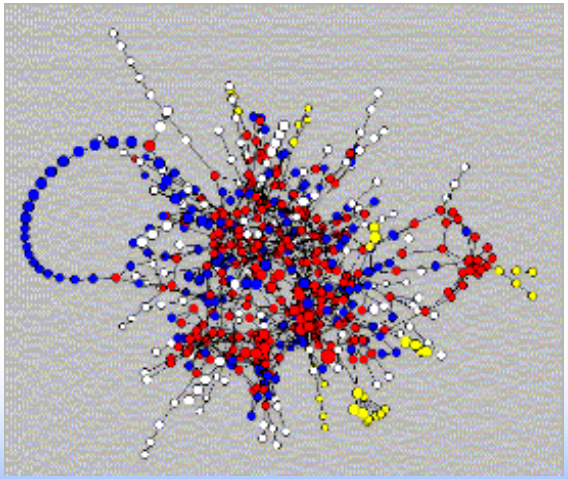




The HPC Enclave

Scientific Results

Experimental Data



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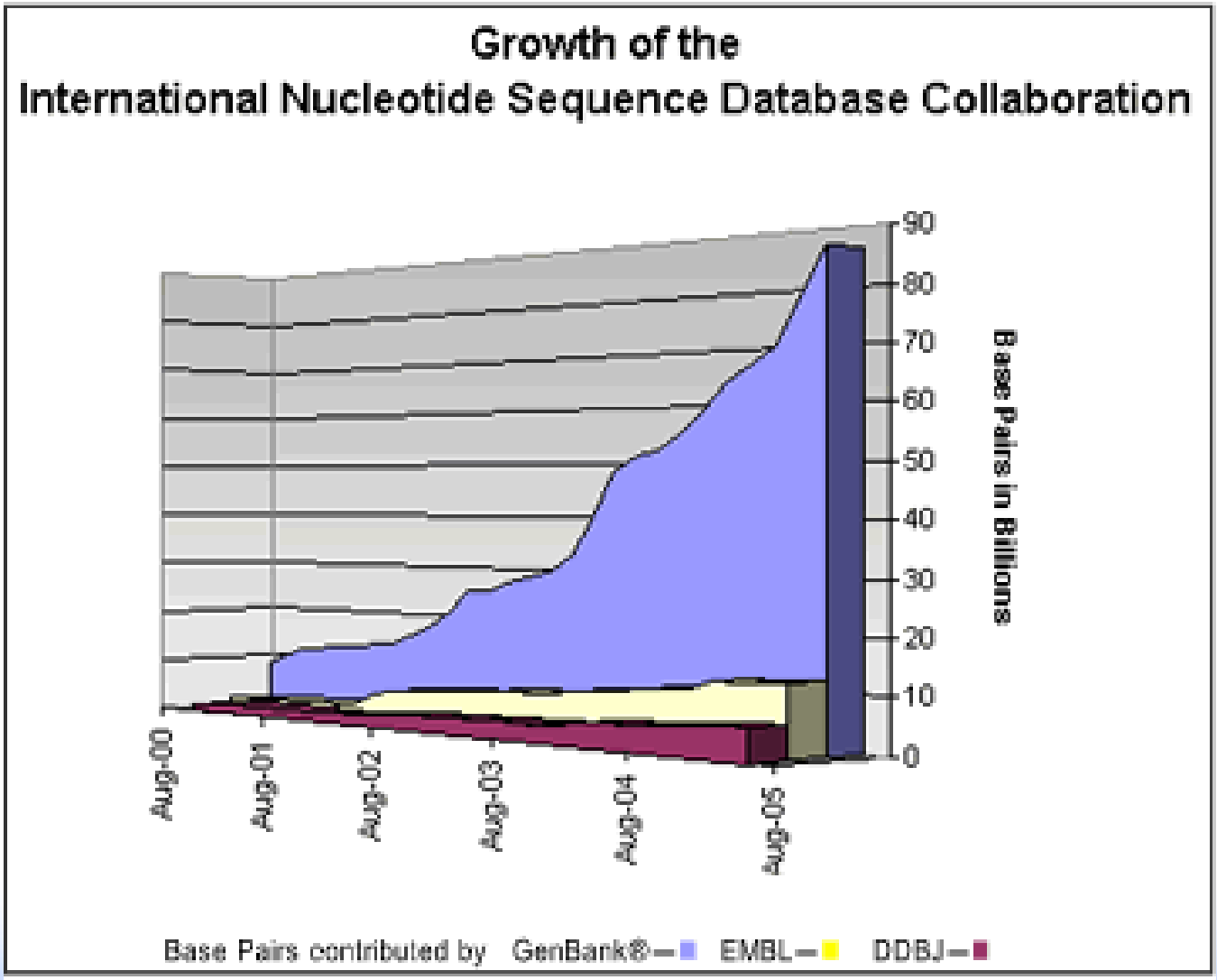

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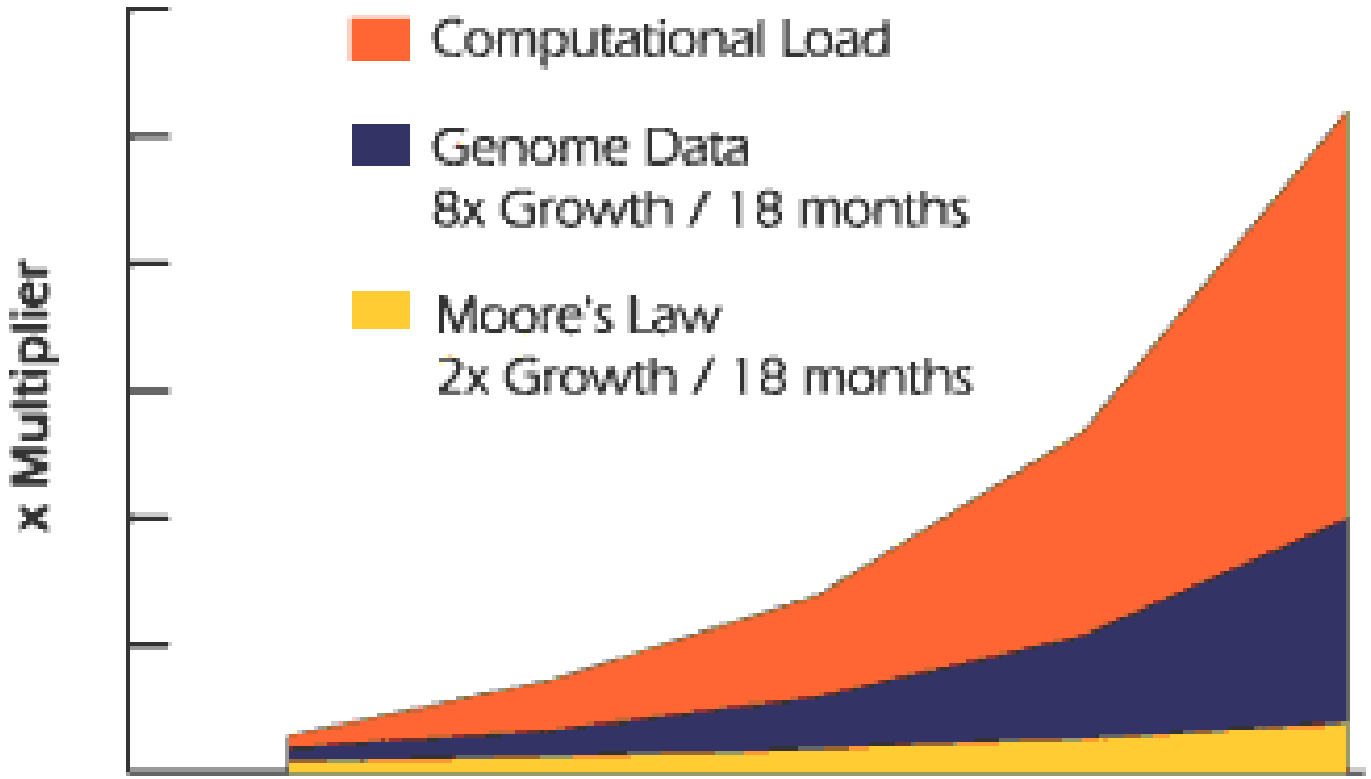
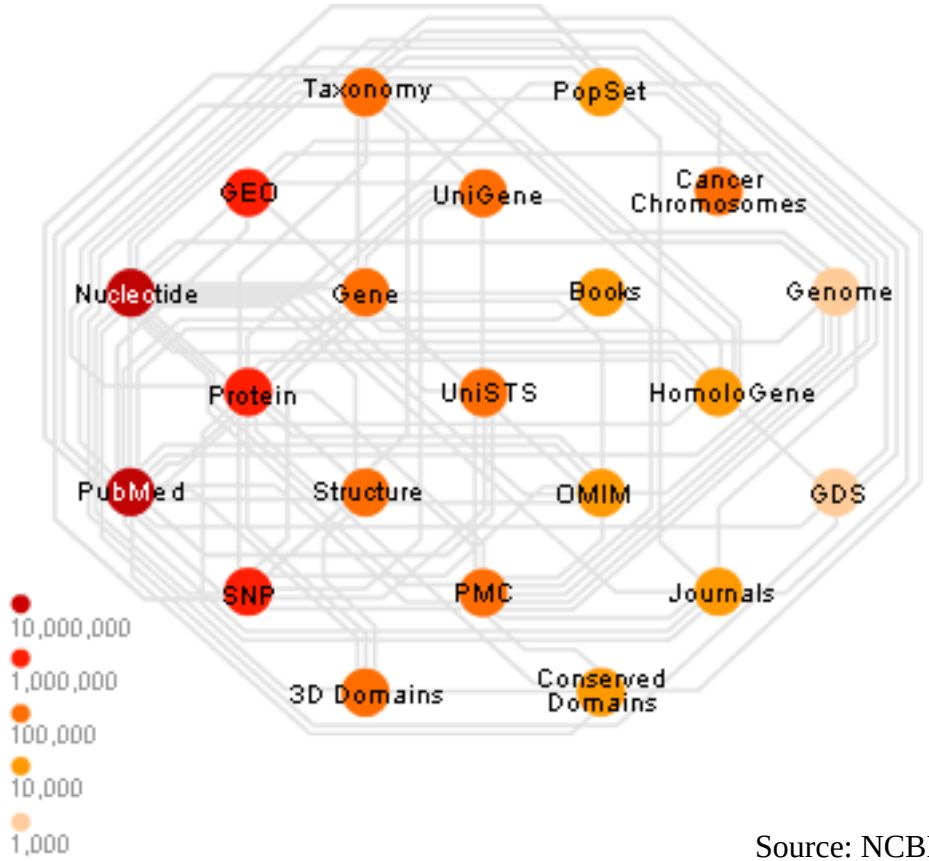
Source: NCBI

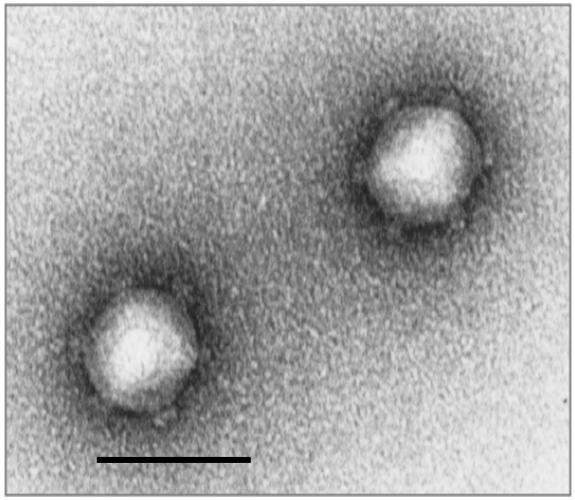


Source: TimeLogic

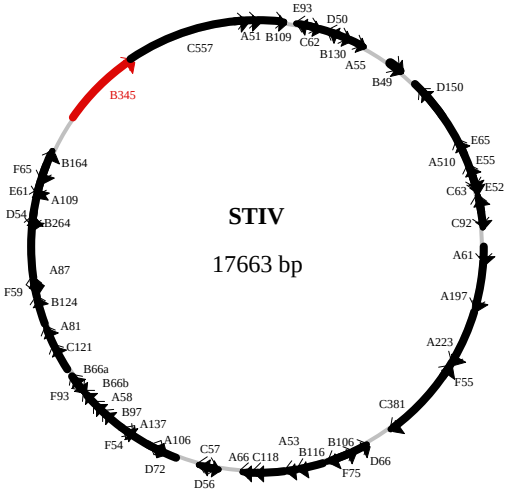
Integration and Relationships between Different Types of Biological Information



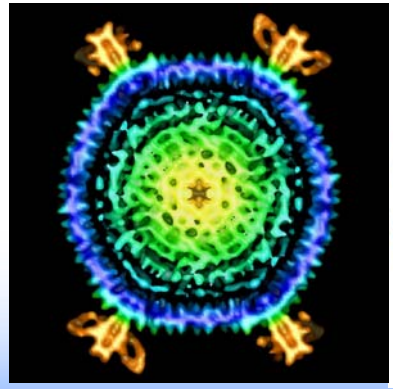
Source: NCBI

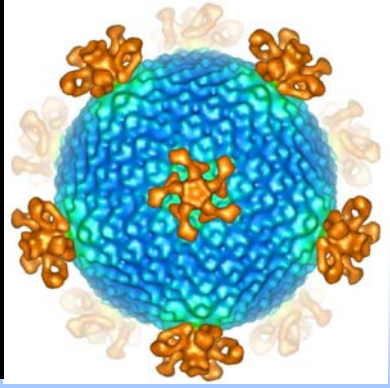


STIV (*Sulfolobus* Turreted Icosahedral Virus) –and other novel thermoacidophilic viruses from Yellowstone



- 17663 bp
- 36% GC content
- 50 ORF's larger than 40 aa
- Largest ORF 138 kD
- Smallest ORF 5.1 kD
- Coat Protein 37.8 kD
- Most viral ORFs are unidentified/hypothetical





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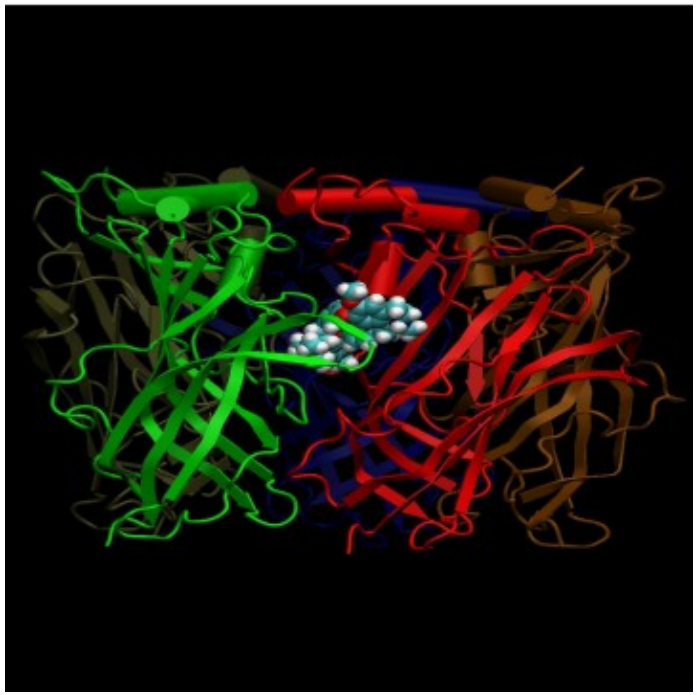
Estimates (Head-Gordon and Wooley, 2001, IBM Systems Journal) for *ab initio* calculation of 100 amino acid protein folding in water (10,000 atoms) exceed 11.5 days for a 100 Tflop machine.



CAMS support for the signature

- Porting, integration and tuning of current bioinformatics tools in the genomics and proteomics “pipelines” (C. Permann)
- Procurement of tailored system in FY06
- Future HPC needs included in outyear planning