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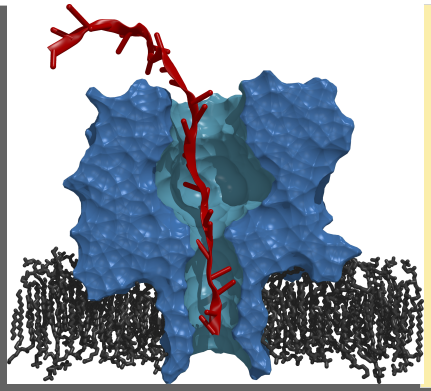
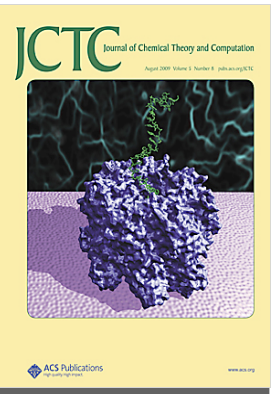
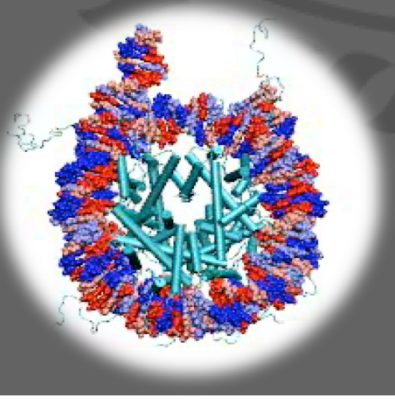


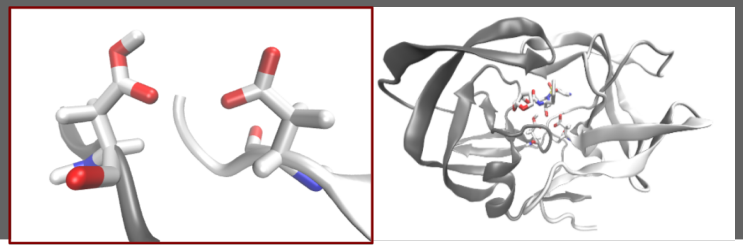


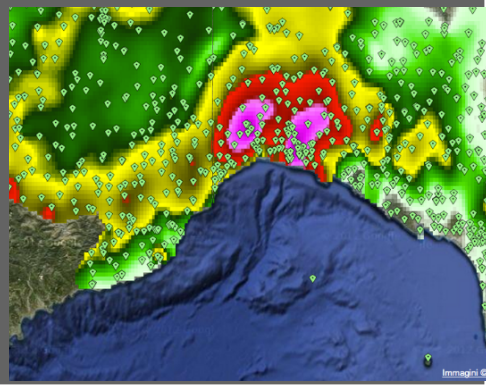
Case Studies of Running Many Simulations on Many Clouds, Clusters and Supercomputers

Shantenu Jha
http://radical.rutgers.edu

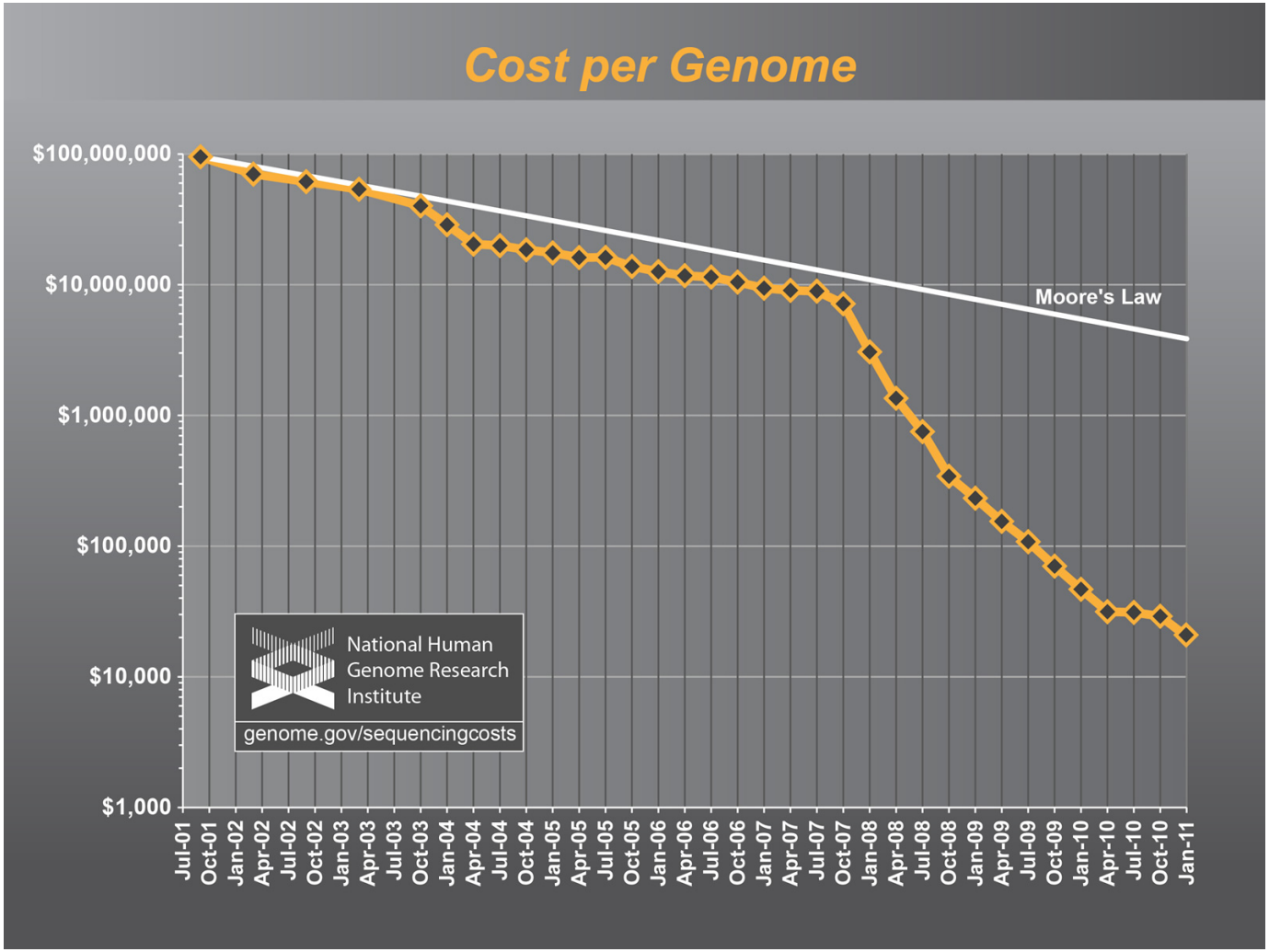
OSDC PIRE, 19th June , 2013







The Challenge of Integrating Compute and Data at Scale



“Many Simulations”: Background and Scenarios

- A Single “Application” is broken into many smaller tasks
  - Naturally decomposed or “by design” (algorithmic and infrastructural)
  - Exploiting parallelism: coarse-grained
- Different types of coupling between these tasks
  - Uncoupled Tasks, Loosely-Coupled Tasks, Sequential Tasks..
- Considerations:
  - “Coupling” general concept for data sharing, synchronization, other dependency
  - Varying rate of coupling between tasks/simulations
  - Regular versus Irregular synchronization:
    - Temporal time
  - Ad hoc pair wise exchange
    - No a priori determined exchange partners
  - Varying task duration: hours to days to weeks

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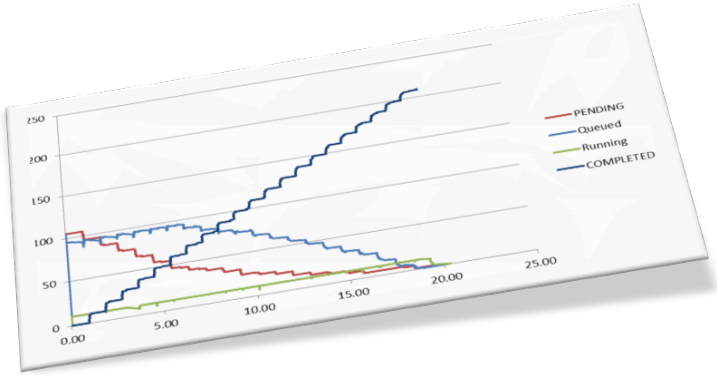
Scalable Online Comparative Genomics of Mononucleosomes

Collaboration with Tom Bishop
Work supported by XSEDE Fellows Grant (Jack Smith)

Current Study of a Sequence



- A Typical “Run”
  - 210 Simulations (5 x 21 x 2)
  - 2400 Cores on Lonestar for ~21 hrs
  - ~50,000 SUs
  - ~750 GB of output
- Total:
  - 10+ Runs (**2100** simulations)
  - 4 Restarts
  - ~500,000+ SUs
  - ~7.5 TB of output

Slide courtesy: Bishop, Smith

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A Pore Man's View of the TeraGrid/XSEDE

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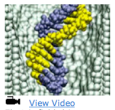
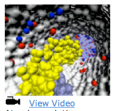
Discovery
New Gene Sequencing Method Could Reduce Cost, Increase Speed

Researchers are developing a new kind of DNA sequencer that will make the dream of "reading" a person's genetic code for less than $1,000 a reality

Double-stranded DNA in a synthetic nanopore revealed by molecular simulation.
Credit and Larger Version



View Video
Electric field-driven transport of double-stranded DNA through a synthetic nanopore.
Credit and Larger Version



View Video
Atomic-resolution description of DNA transport through a synthetic nanopore.
Credit and Larger Version

July 16, 2010

The first human genome took 13 years and $3 billion to sequence. Today, geneticists can generate the same information in a matter of months, for a fraction of the cost.

As "next-generation" gene sequencers begin to make their mark on the life sciences, teams around the world are racing to develop new and improved DNA sequencers that can ingest a strand of nucleotide bases and directly "read" a person's genetic code for less than $1,000.

The medical community predicts that the advent of the $1,000 personal genome will lead to major changes in the understanding and treatment of illness. Researchers will be able to perform widespread comparative studies to correlate disease to gene expression. Chemists will design genetically-targeted drugs, and doctors will deliver medical treatments based on a patient's

About the Cover

August 11, 2009: Vol. 5, Iss. 8

An external view of the alpha-hemolysin protein pore (light blue) on a lipid bilayer (light purple). A 25 base adenine polynucleotide (green) is beginning to translocate through the pore. The molecular conformations of the protein and polynucleotide have been extracted from molecular dynamics simulations. See H. S. C. Martin, S. Jha, S. Howorka, and P. V. Coveney, p 2135. View the article.

Go to:

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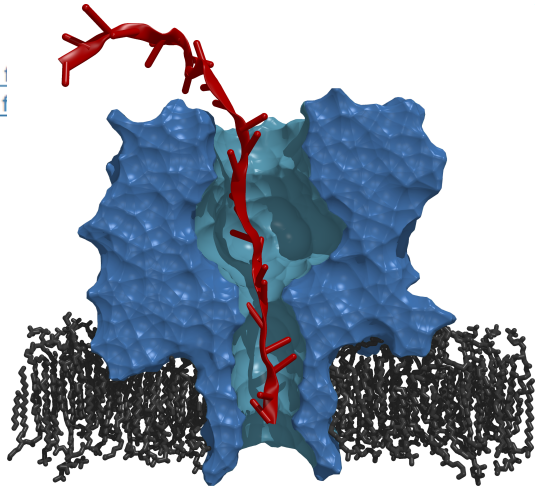
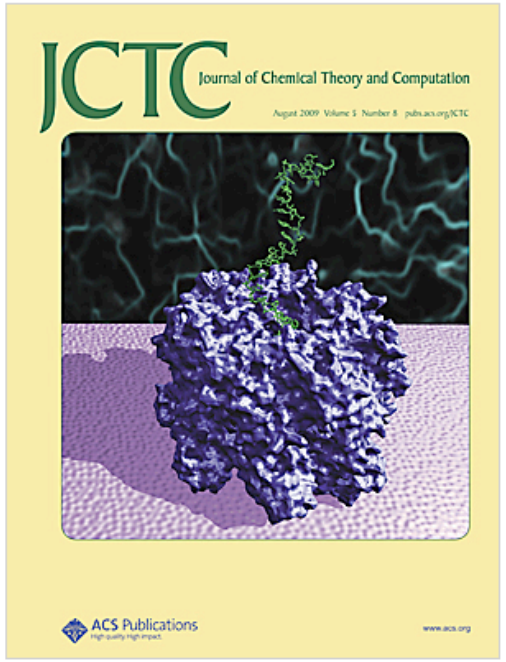
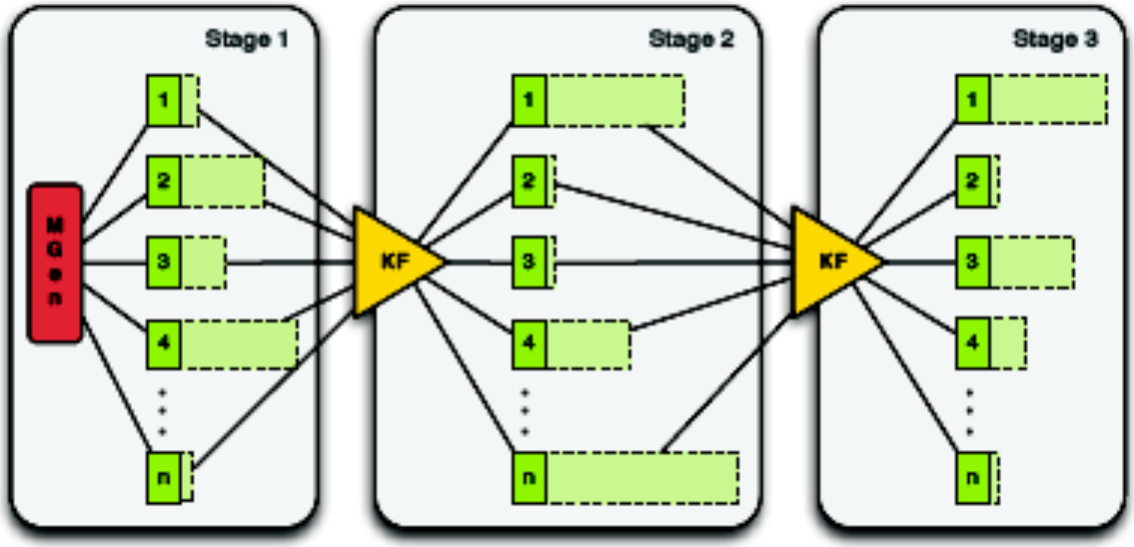
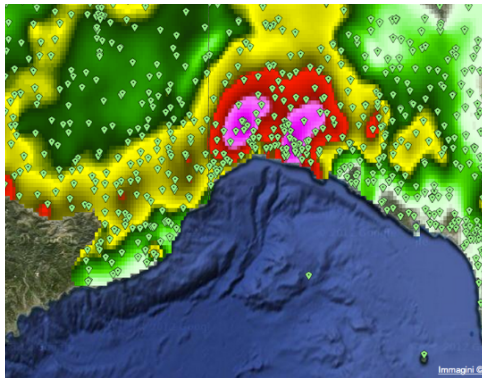
» Cover Art Gallery



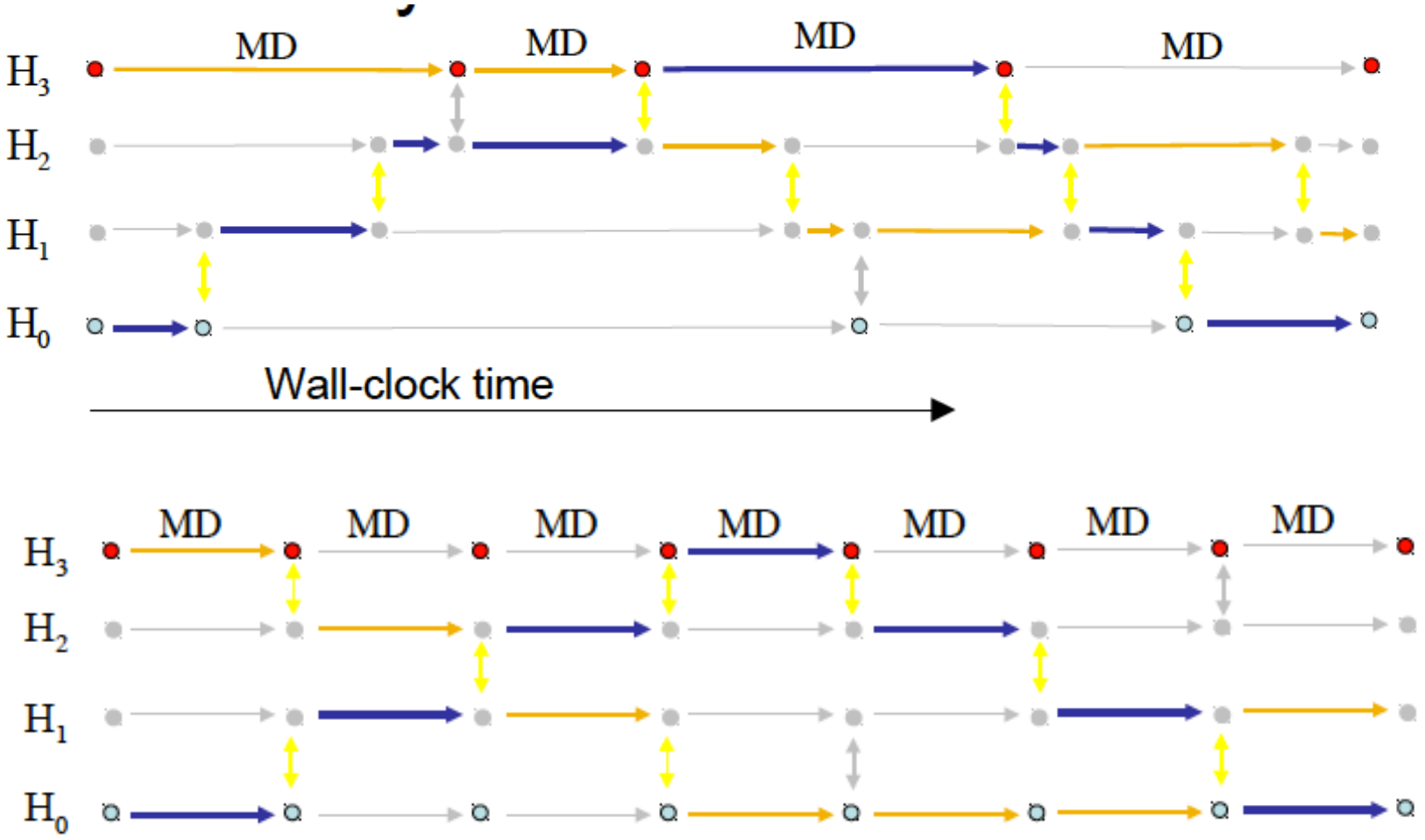


Regular Synchronization





Irregular Synchronization



Scenarios: Redux

- Different types of Coupling
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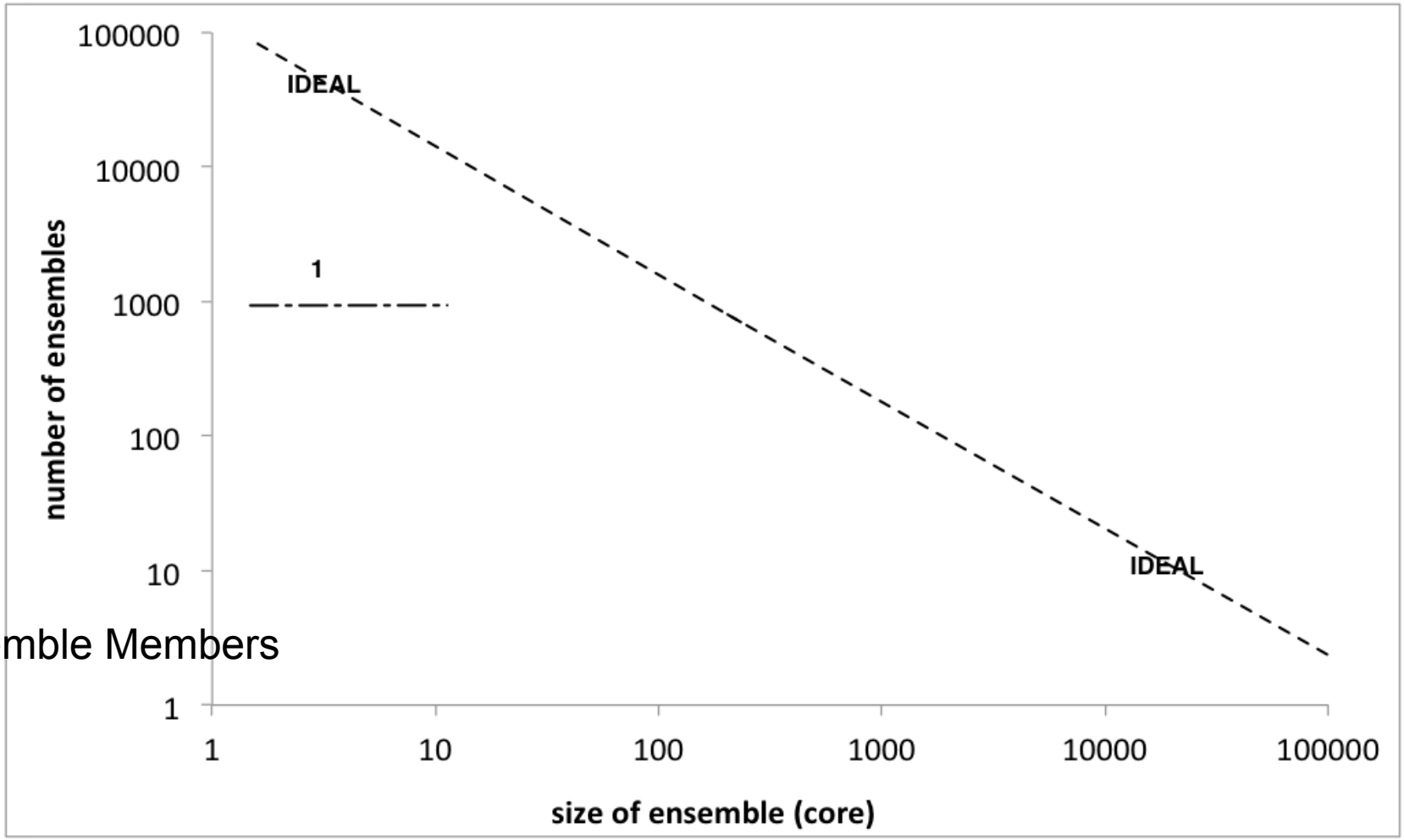
“Slice and Dice” Resources



# of Ensemble Members

Number of cores per Ensemble Member

Scaling Along Many Dimensions

- Scaling Dimension #1: Size of each task
  - *Scale-up*
  - 1 core per task, 128 cores per task..
- Scaling Dimension #2: Total Number of Tasks
  - *Scale-Out*
  - Enhanced Sampling in molecular simulations O(1000), statistical errors O(10^6),…
- Scaling Dimension #3: Number of Resources Used
  - *Scale-Across*
  - Execute on Clouds, Clusters, Supercomputers
- Scaling Dimension #4: Total Number of Tasks/per unit time
  - Real time processing

Summary

- Many science and engineering problems can be naturally expressed
  - Ensembles, loosely-coupled, “constructing” workflows
- Advantages:
  - Scalable Access to more resources
  - Efficient, Effective, Dynamic resource management
- Challenges:
  - How to manage coordination across many tasks?
  - Responding to dynamic resource: How?
  - Distributed Failures, Heterogeneity and Interoperability:
- Beyond simple, static, single execution: Well engineered tools built using the appropriate abstractions
  - Compute capacity is fluctuating, growing/shrinking

References

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  - http://github.com/saga-project/BigJob/wiki
- RADICAL:
  - http://radical.rutgers.edu/
- Publications:
  - http://radical.rutgers/edu/publications

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- ``**P*: A Model of Pilot-Abstractions"**, 8th IEEE International Conference on e-Science 2012 (DOI: 10.1109/eScience.2012.6404423)

- *"***Distributed Computing Practice for Large-Scale Science & Engineering Applications"** *Shantenu Jha, Daniel S. Katz, Jon Weissman* et al, Computing and Concurrency: Practice and Experience, 2012 (DOI: 10.1002/cpe.2897)

- **"Pilot-Data: An Abstraction for Distributed Data"**, arXiv:1301.6228