Computational Science & Engineering
Building a Community
(SIAM SIAG for CSE)

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Outline

IBM Research

- Brief background why CSE is important
- Comment on Computational Scientists
- Overview of the SIAM SIAG CSE Organization
- Comments on CSE and its implications wrt to changing HPC landscape
- Closing Remarks

Future Foresight and Right Action

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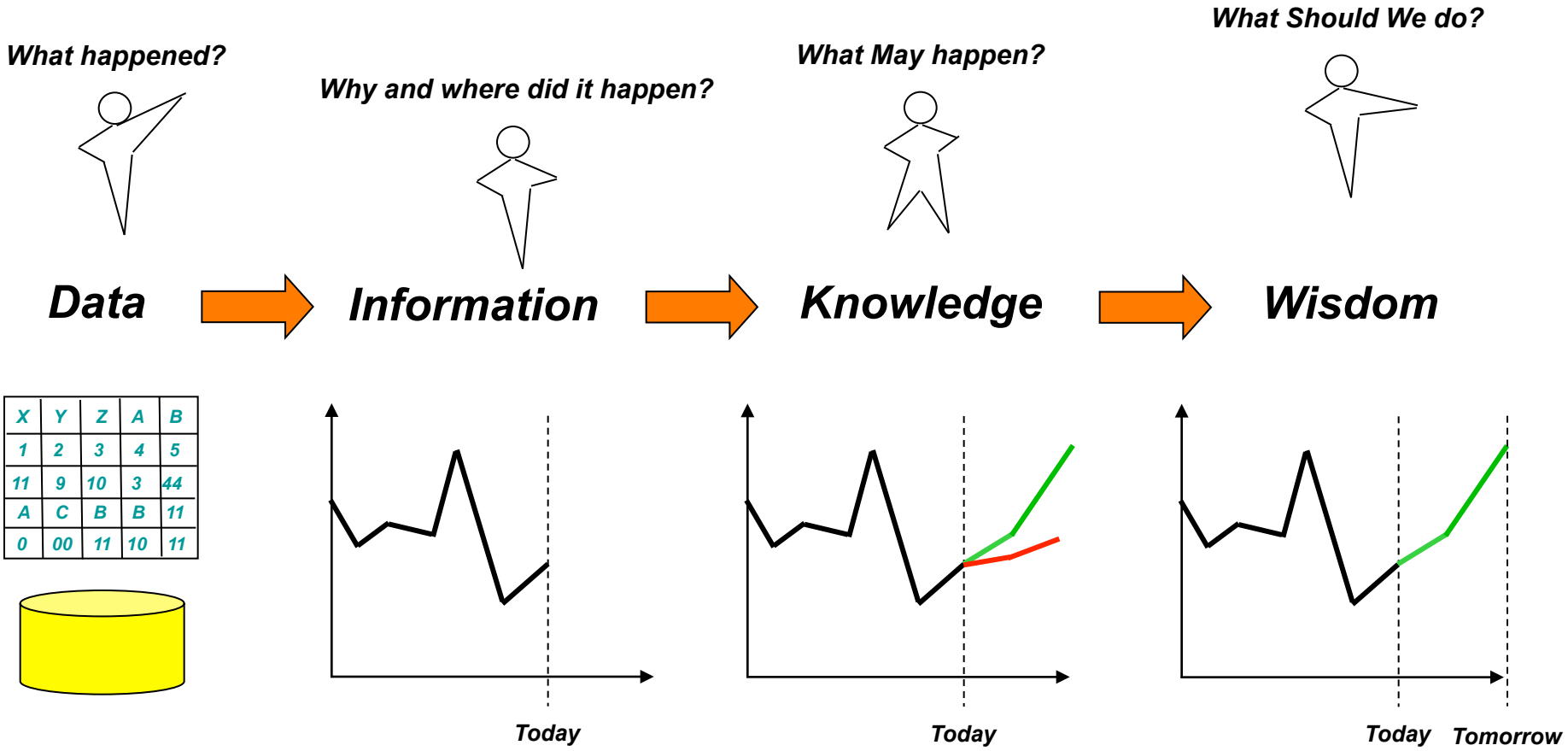

Simulation & Modeling

The Emerging Framework for XXI Century Science & Technology Innovation

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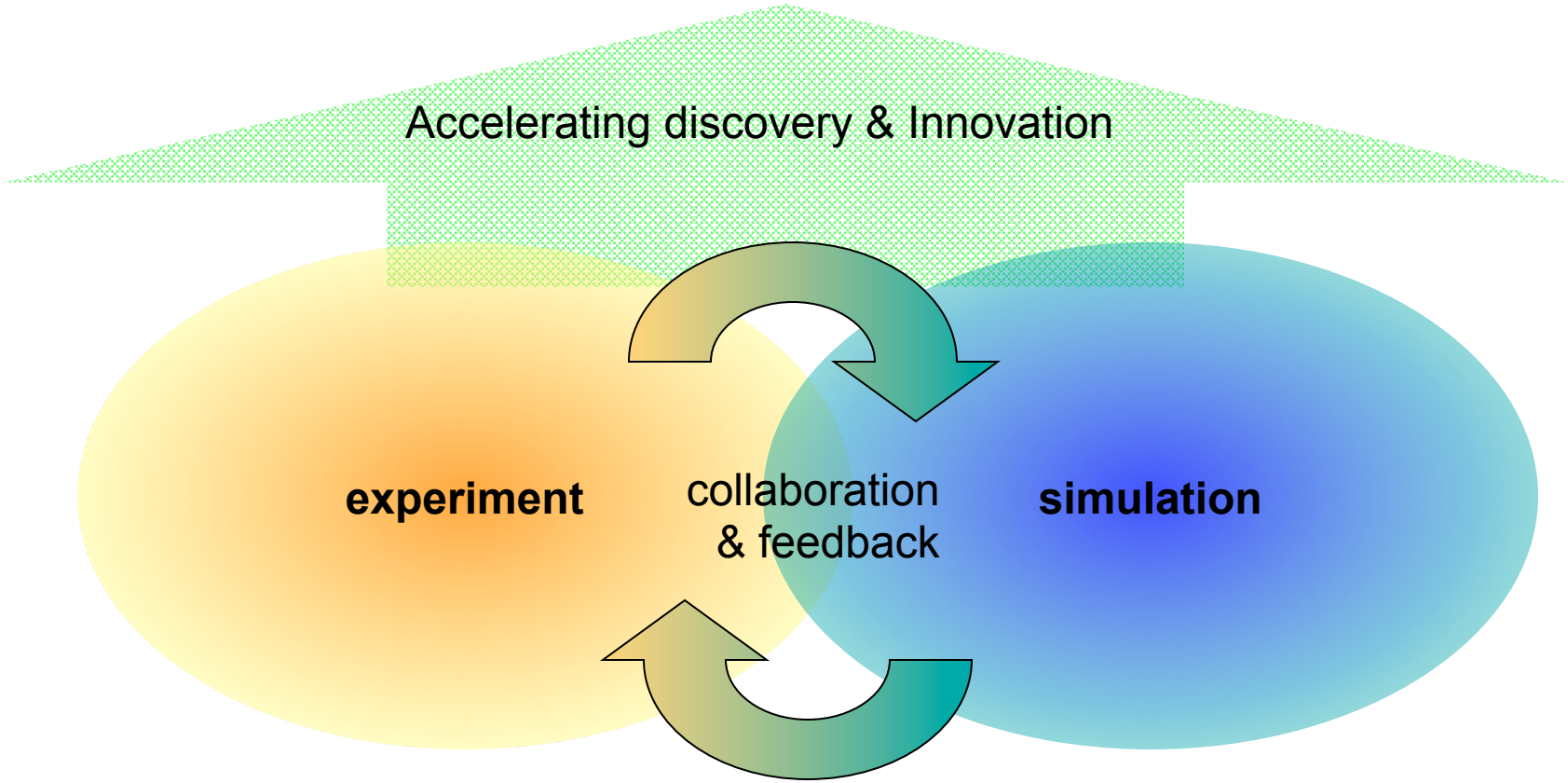
Materials Science | Energy | Engineering | Climate & Environment | Life Sciences



EXASCALE REQUIRED

Computational Science and Engineering
Simulation Based Engineering Sciences (SBES)

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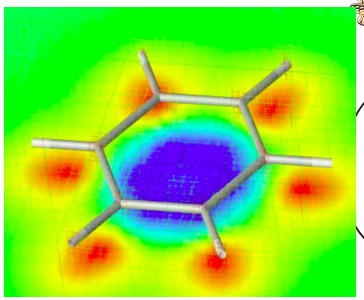
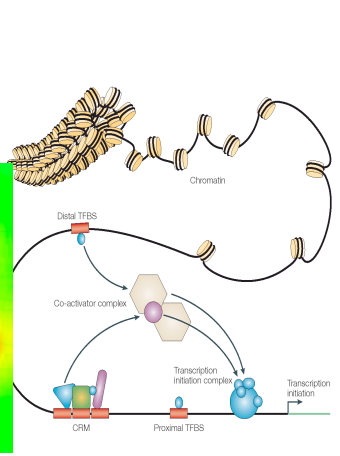
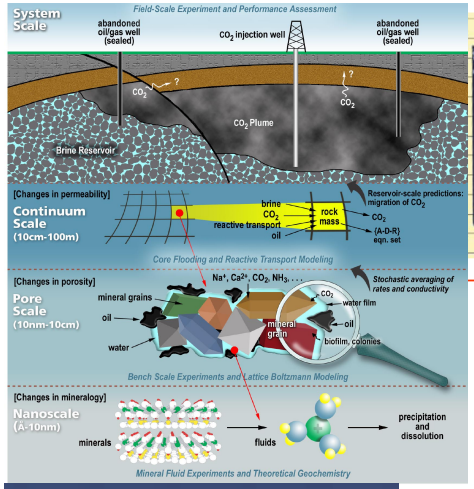
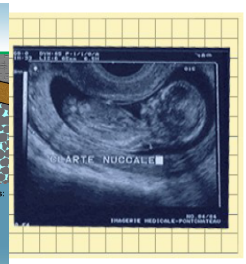
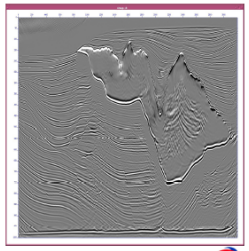
- Apply computational science techniques in various areas – multi-scale & multi-”physics” to advance the next generations of computing
  - Computational and Systems Biology
    - Tumor & heart modeling
    - Transcription factor binding site id
    - Imaging – medical (& other)
  - Geoscience
    - Reservoir & groundwater
    - Wave propagation
    - Atmospheric & ocean modeling
  - Computational Fluids & Structures
    - Reactive flows
    - Convective flows
  - Advanced numerical techniques, High-end visualization, combined systems
    - Multi-resolution Wavelets
    - High order splines
    - Multi-Grid
    - Hybrid computing

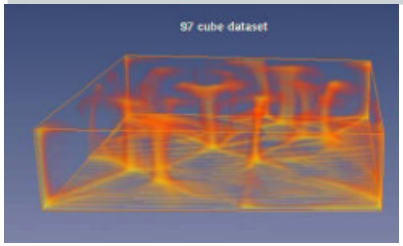


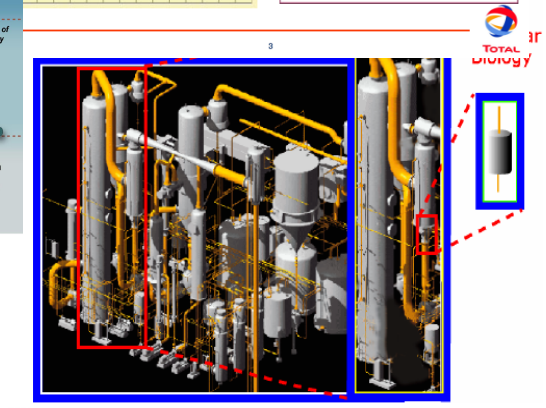












SIAG/CSE OFFICERS 2011-2012 CONTACTS (Elections to be held this Fall – new Officers 2013)

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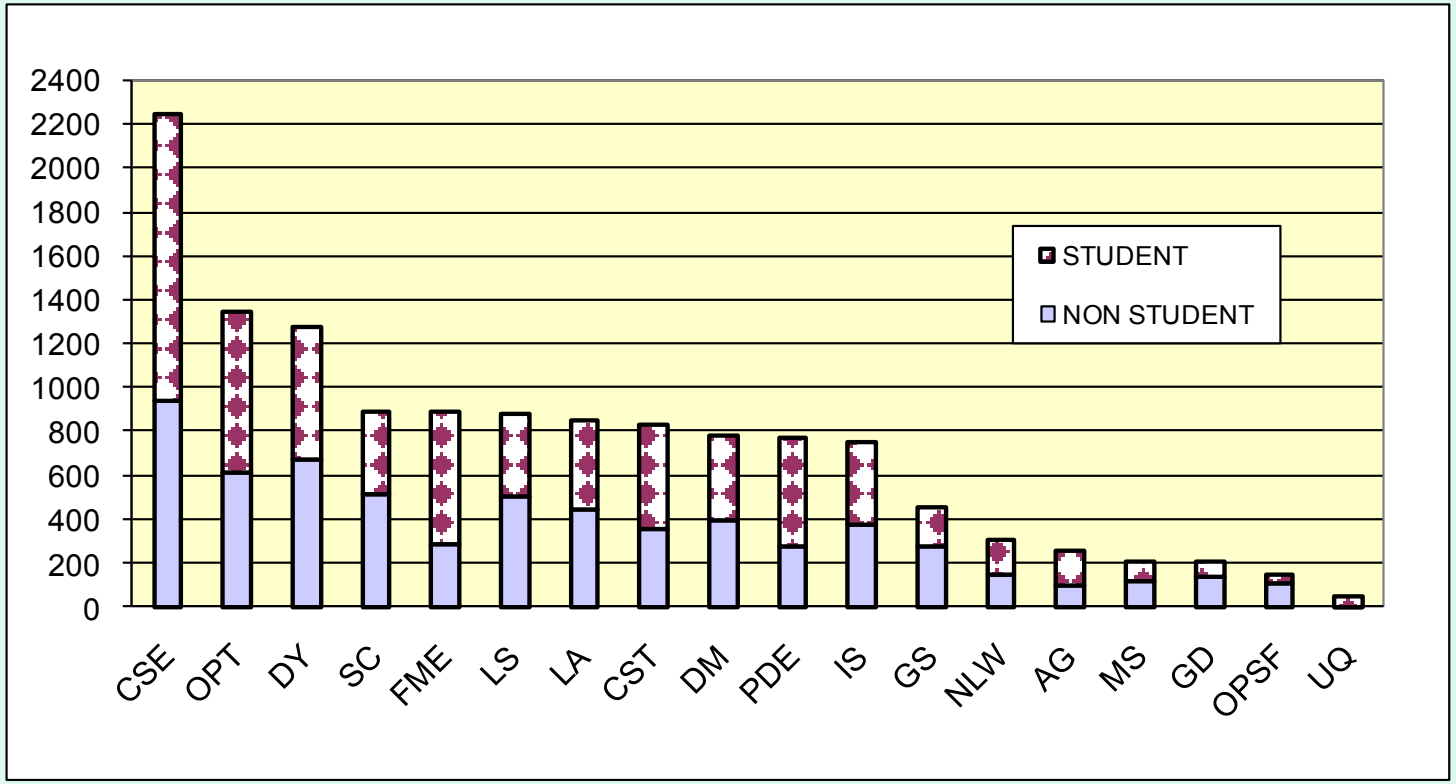
Chair:	Kirk Jordan
	kjordan@us.ibm.com
Vice Chair:	Carol Woodward
	cswoodward@llnl.gov
Program Director:	Karen Willcox
	kwillcox@mit.edu
Secretary/Treasurer:	Luke Olson
	lukeo@illinois.edu

ACTIVITY GROUP MEMBERSHIP 12/31/10

47% non-students and 66% students belong to a SIAG



Membership History

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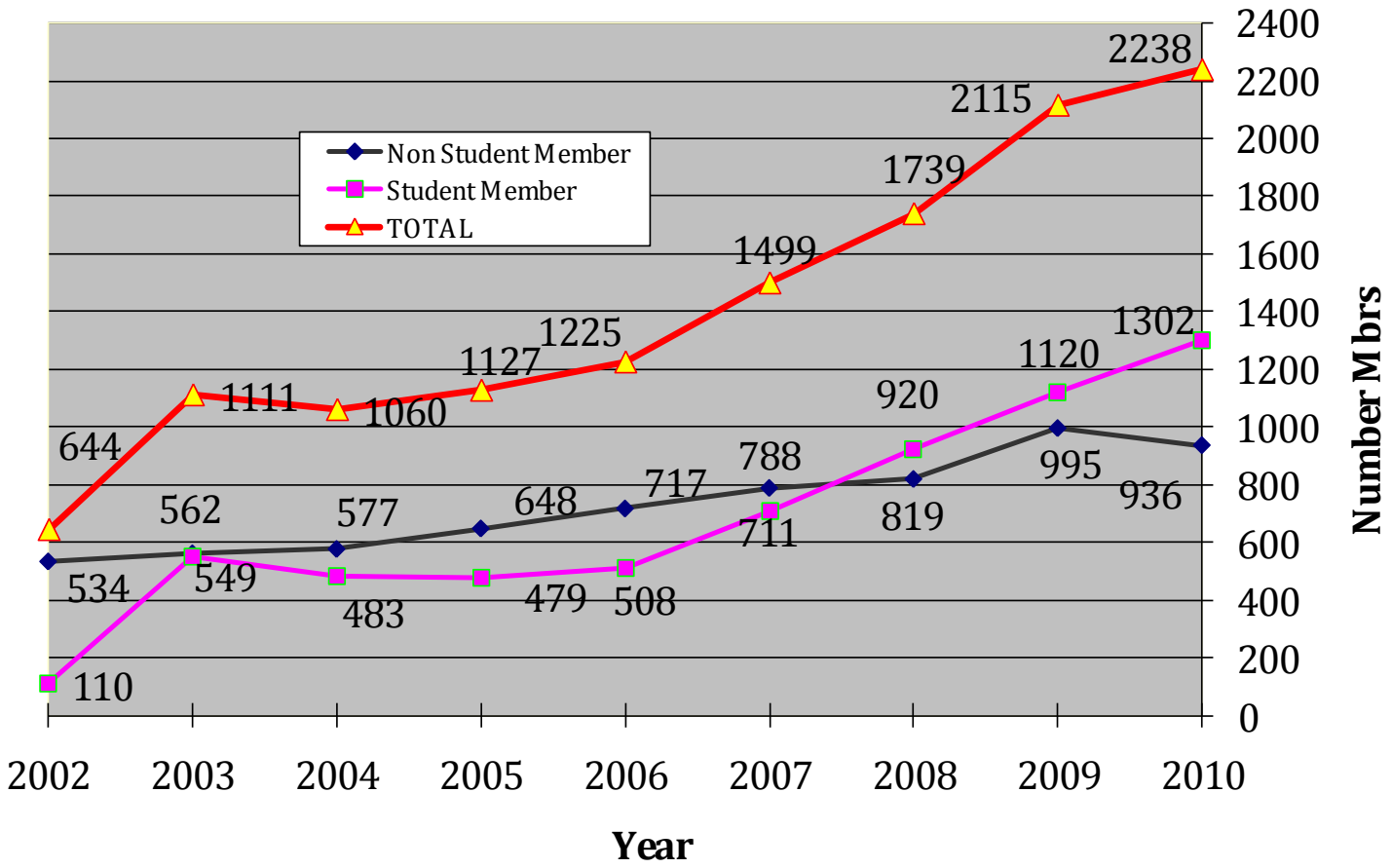
Membership History as reported at the last CSE Business Meeting - 2011



End of 2011 - 11.5% from 2115 members in 2009 to 2359

SIAG/CSE MEMBERS

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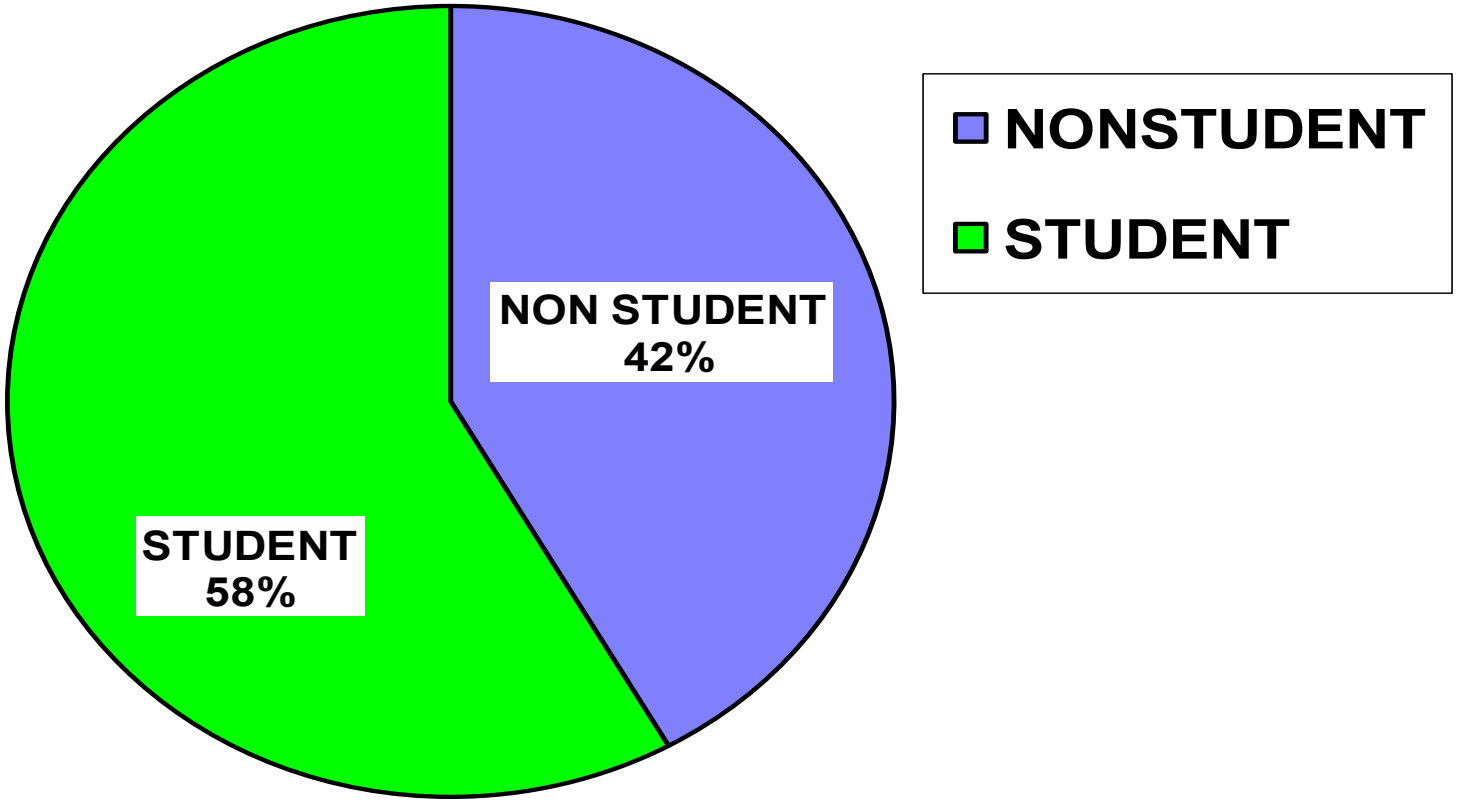

Students membership is free – accounts for large number

Need to convert student members to full members

SIAG/CSE MEMBERS BY EMPLOYER TYPE
not including students

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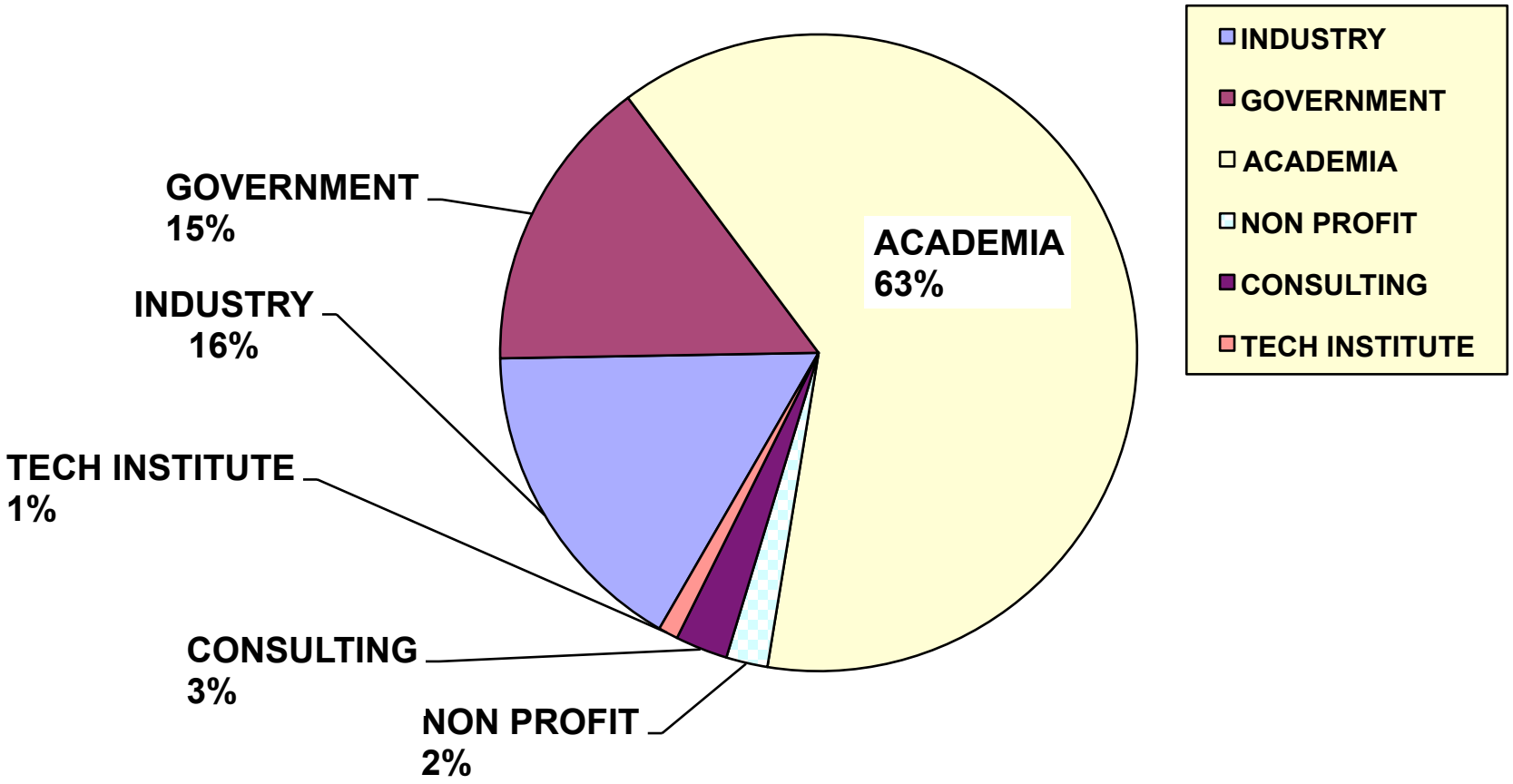

SIAG/CSE MEMBERS BY GEOGRAPHY

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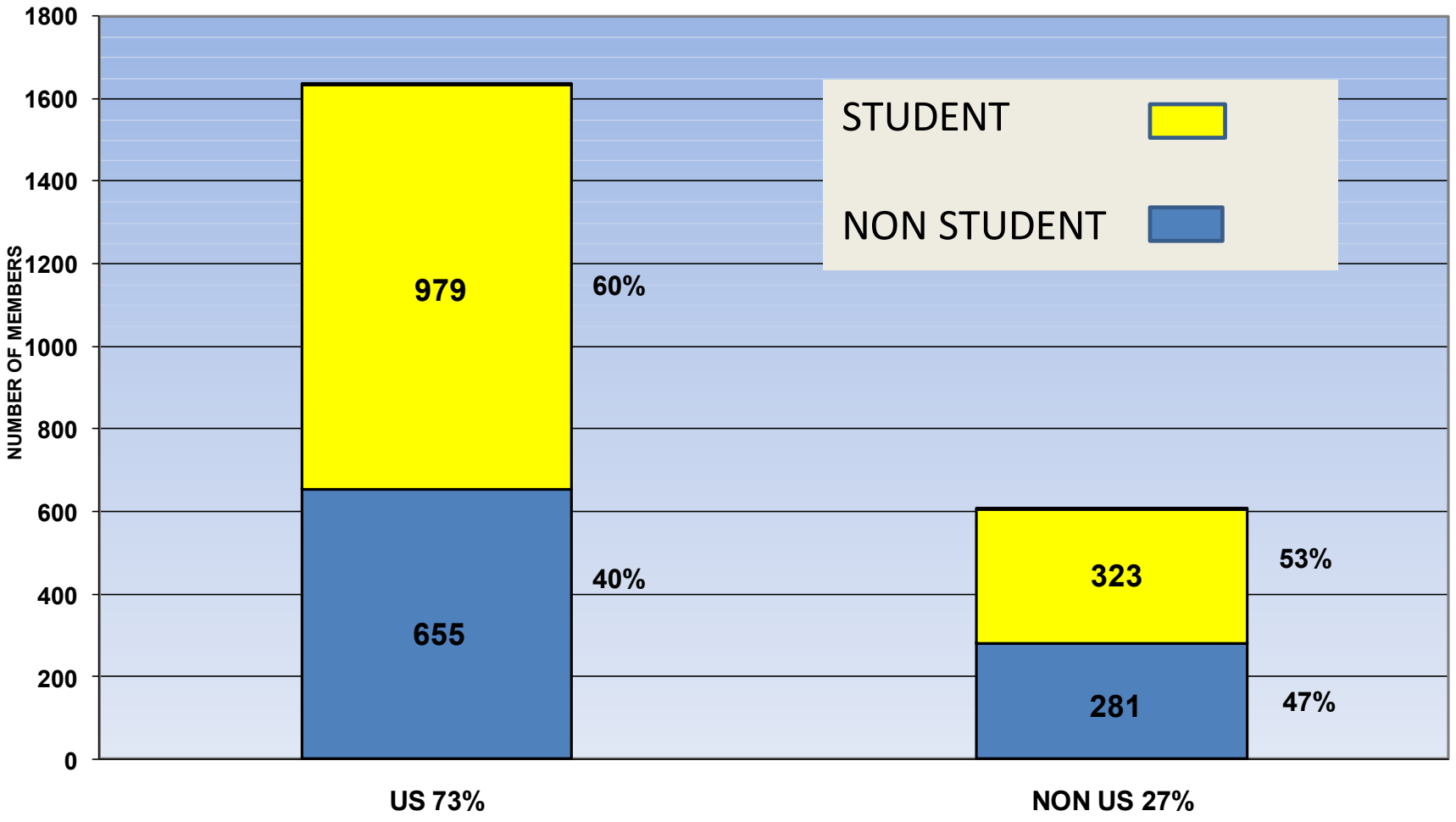

GAMM CSE could help increase the non-US members – goal of 65-35 %

SIAG/CSE MEMBERSHIP BY GENDER
MALE 85% FEMALE 15%

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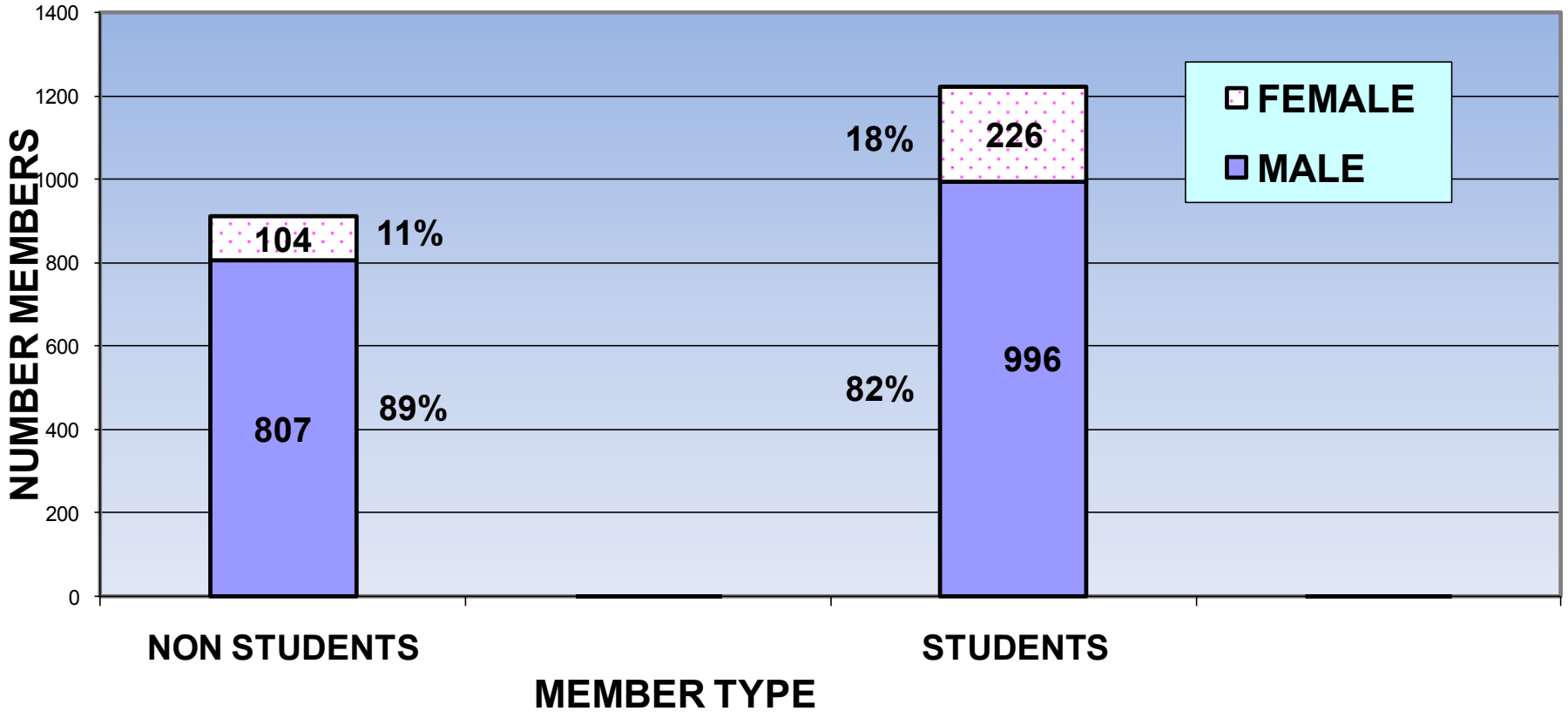

Female membership remains at around 11%, however over 18% of the students are female.

Break down by Departments

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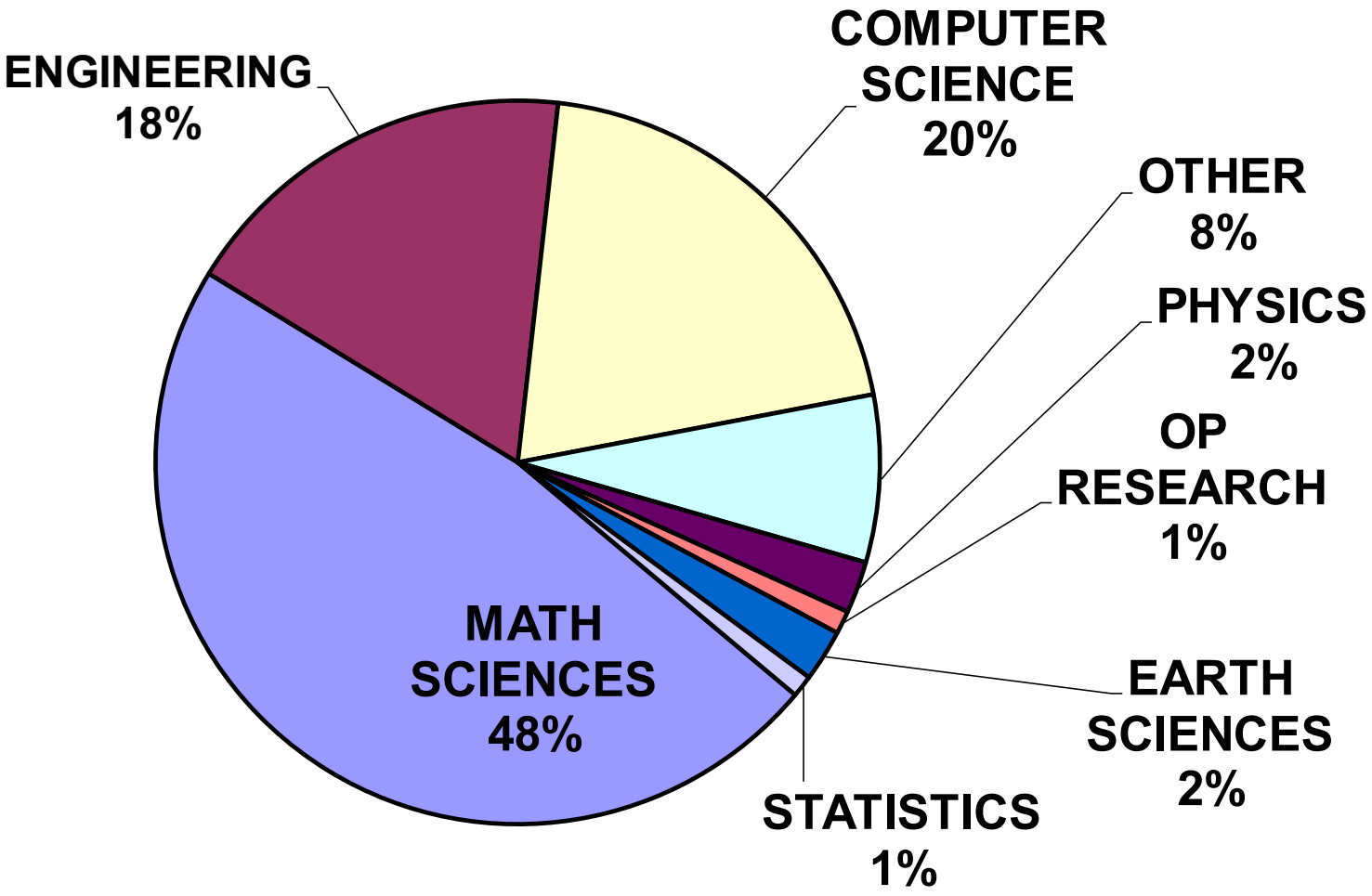

Latest Updates

IBM Research

- **SIAG Charter renewed through 2014 – Charter renewed at Annual Meeting – July 2012.**

- **SIAG Elections in 2012:**
  - Nominating committee put together list of 8 excellent candidates – 2 per office.
  - SIAG CSE members vote this fall.

- **Electronic Resources**
  - **Moderated** Mailing List: siam-cse@siam.org
  - Wiki: http://wiki.siam.org/siag-cse/
  - SIAG/CSE website: http://www.siam.org/activity/cse/

CONFERENCES

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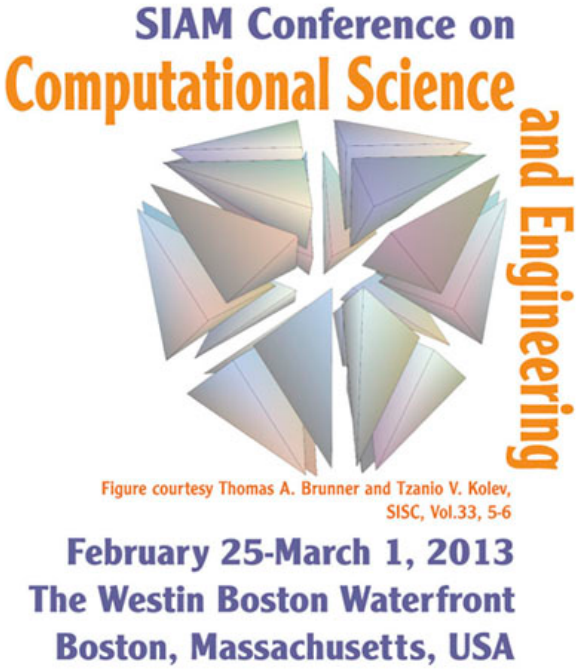
- **ICIAM July 18-22, 2011 - Vancouver, British Columbia, Canada**
  - SIAG CSE officers helped organize a series of Industrial Minisymposia
  - 14 minisymposia partially organized by the CSE SIAG
    - Finance and Risk Management - 6
    - Imaging and Inverse Problems- 6
    - Graduate Research Internships with Industry - 2

- **SIAM CSE 13, Boston, USA - February 25 – March 1, 2013**
  - Co-Chairs - Karen Willcox & Hans Petter Langtangen
  - Themes:
    - Multiphysics and Multiscale Computations
    - Identification, Design, and Control
    - Surrogate and Reduced-order Modeling
    - Verification, Validation, Uncertainty Quantification
    - Discrete Simulations
    - Scientific Data Mining
    - Scalable Algorithms for Big Data
    - Simulations on Emerging Architectures
    - Exascale Challenges
    - Scientific Software and High-Performance Computing
    - Applications in Science, Engineering, and Industry
    - Computational Mathematics of Planet Earth
    - CSE Education



- **Organize CS&E tracks or minisymposia at 2014 SIAM Annual Meeting**
  - **Ideas on topics & Opportunity for GAMM-FA CSE**

Trends in Computing Performance

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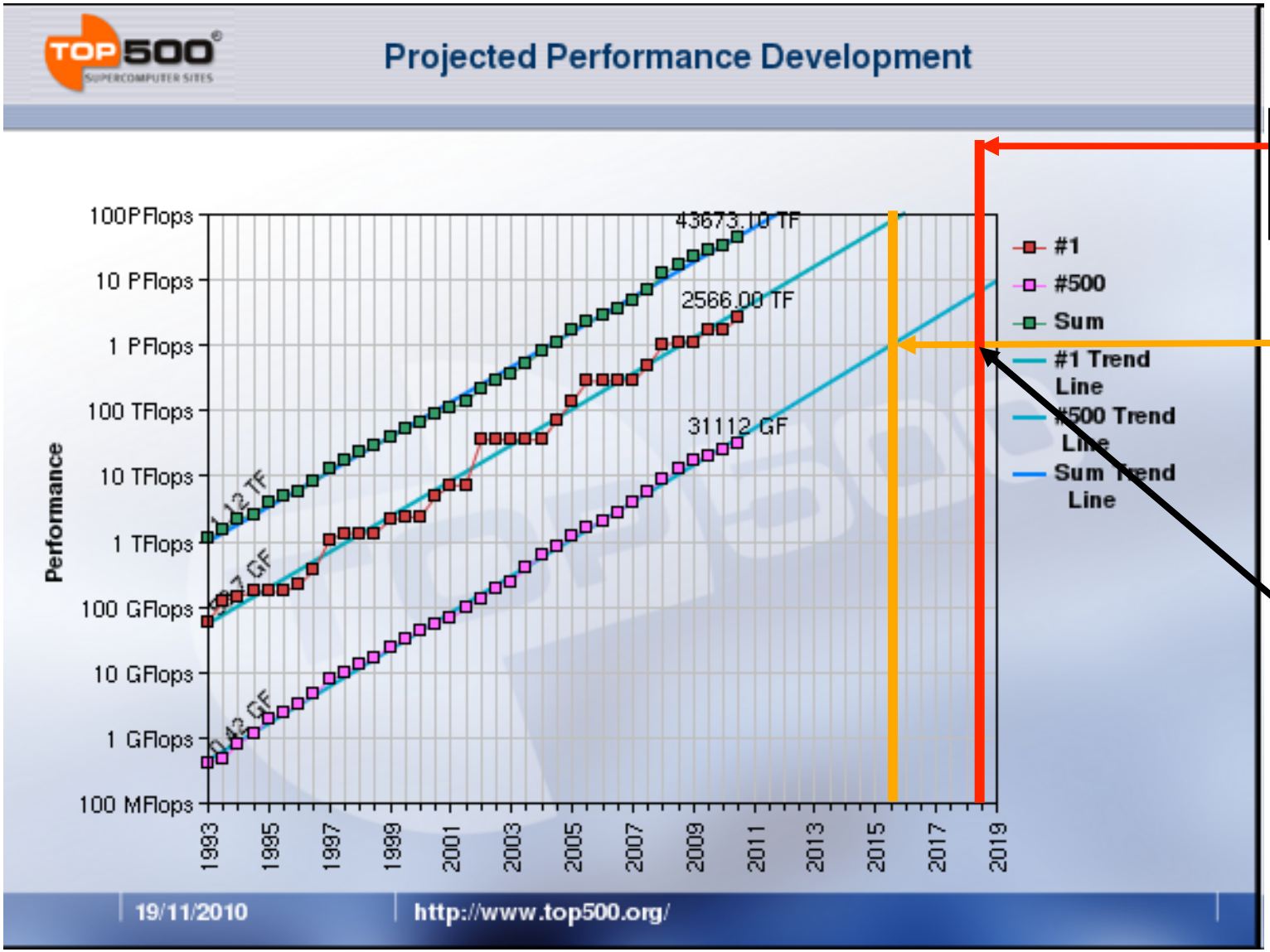

1EFlop ~2nd half of 2018 – est cost $200M

1PFlop ~2nd half of 2015 is bottom of Top500

1PFlop ~2nd half of 2018 – est. cost < $200K

Application Characterization Snapshot from Blue Gene / Q

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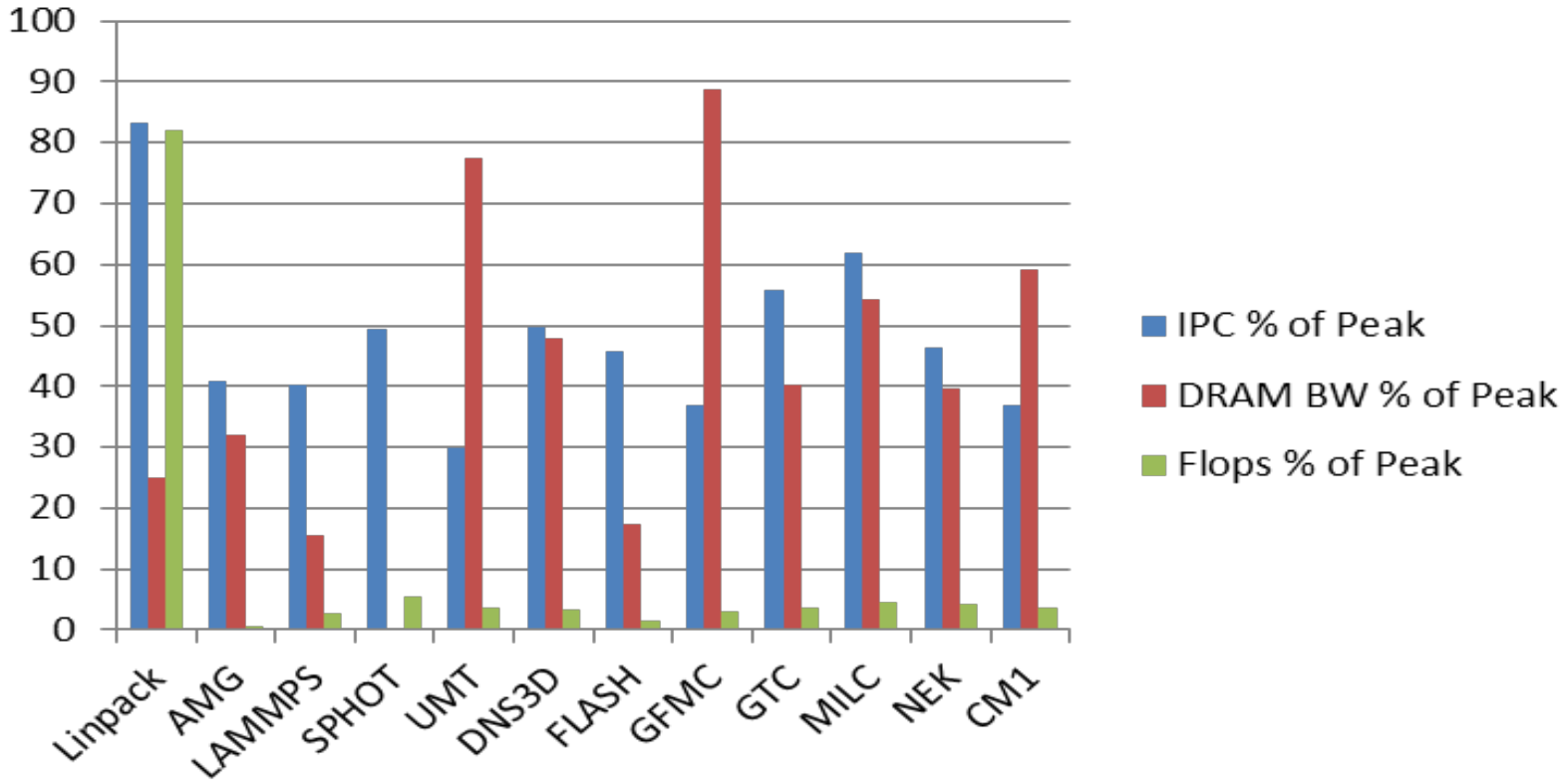

- This data was obtained on a prototype Blue Gene / Q rack.
  - AMG, LAMMPS, SPHOT, UMT are NNSA (Sequoia) benchmarks
  - DNS3D, FLASH, GFMC, GTC, MILC and NEK are Office of Science (ANL) applications.
  - CM1 is a weather / climate app from NCAR
- Even within these three simple metrics, balances are significantly different for different applications.
  - Linpack is a clear outlier
  - Apps except Linpack have low fraction of floating point peak
  - Apps except Linpack have many integer instruction for each floating point operation
  - Main memory bandwidth requirements differ significantly between apps.

Implications of Peta & Exascale Applications

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- Need for scalable, parallel, robust, optimal methods for:
  - Advanced discretization in time & space
  - Adaptive mesh/order refinement/coarsening methods
  - Fast solvers that address nonlinearities, multiphysics couplings, anisotropies, heterogeneities
  - Inverse problem & data assimilation
  - Uncertainty quantification – forward propagation and inverse estimation
  - Optimization under uncertainty

- At this point fair to say:
  - Some limited progress in designing/implementing optimal methods for 1st three that scale to $O(10^4)$ to $O(10^5)$ cores
  - Last three in infancy, even for model problems
  - Many current methods intractable for last 2 for peta/exascale applications

- Need for good Computational Science & Engineering skills

Courtesy Omar Ghattas

Smarter Planet

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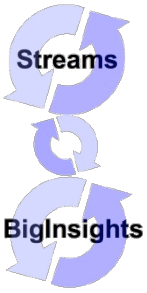
Data Centric Computing

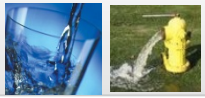
+



Reactive + Deep Analytics Platform

Systems, Services and Solutions Ecosystem

DeepWater
Water management



DeepCurrent
Power Delivery

DeepEyes
Webcam Fusion

DeepTraffic
Area Traffic Prediction

DeepSafety
Police/Security

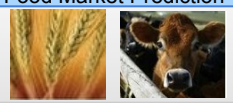
DeepFriends
Social Network Monitor

Let's build a smarter planet

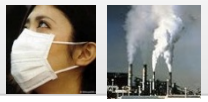
DeepSoil
Farm Prediction

DeepPulse
Political Polling

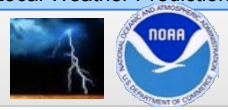
DeepBasket
Food Market Prediction



DeepBreath
Air Quality Control



DeepThunder
Local Weather Prediction



DeepResponse
Emergency Coordination

Summary – Computational Science & Engineering

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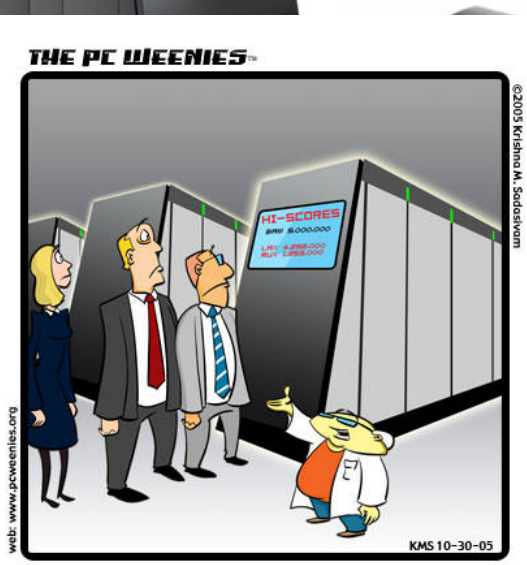
- Next 10 years:
  - HPC Capability evolving - will impact CSE and vice versa
    - Fidelity and time to solution relevant for industrial / commercial use
    - Hardware costs continue to fall
  - Focus shifting from Hardware to Solutions
    - Expertise now critical – CSE expertise will drive the solutions
    - Economic opportunity is in development and delivery of robust solutions and services

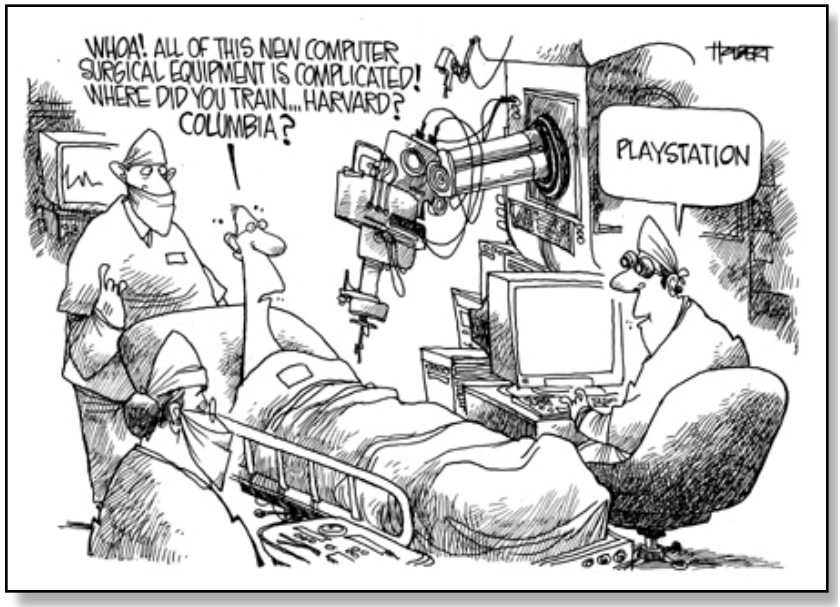
- Opportunity for many but CSE in particular
  - Brand New, Green Field Landscape!
  - Focus shifts from single applications to solutions and services
  - Significant opportunities for entry of new players
  - Economic impact is critical

Summary – Cont.

- A time of significant challenge
  - Just as HPC starts to have real scientific and industrial impact - it gets extraordinarily hard.
  - Algorithmic development needed – i.e. Math, and CSE play important roles
  - Validation & Verification and Uncertainty Quantification required – i.e. More Math & CSE
- A radical research and development approach required – CSE major role
  - Multidisciplinary from domain science, math formulation, algorithms to system design
  - Collaboration essential from systems to applications
  - Collaboration on industrial / commercial workflows
- We will have succeeded when
  - we stop talking about architecture
  - we focus on real impact: Research, Industry, Business
- The answers remains left to the audience/the reader/the users - - US!!



"OUR SUPERCOMPUTER IS CAPABLE OF PERFORMING TRILLIONS OF COMPUTATIONS PER SECOND, BUT WE PRIMARILY USE IT FOR BIT TORRENT AND GAMING."



In the end, it's not about the technology; It's what you do with it that counts (Computational Science & Engineering will Impact)

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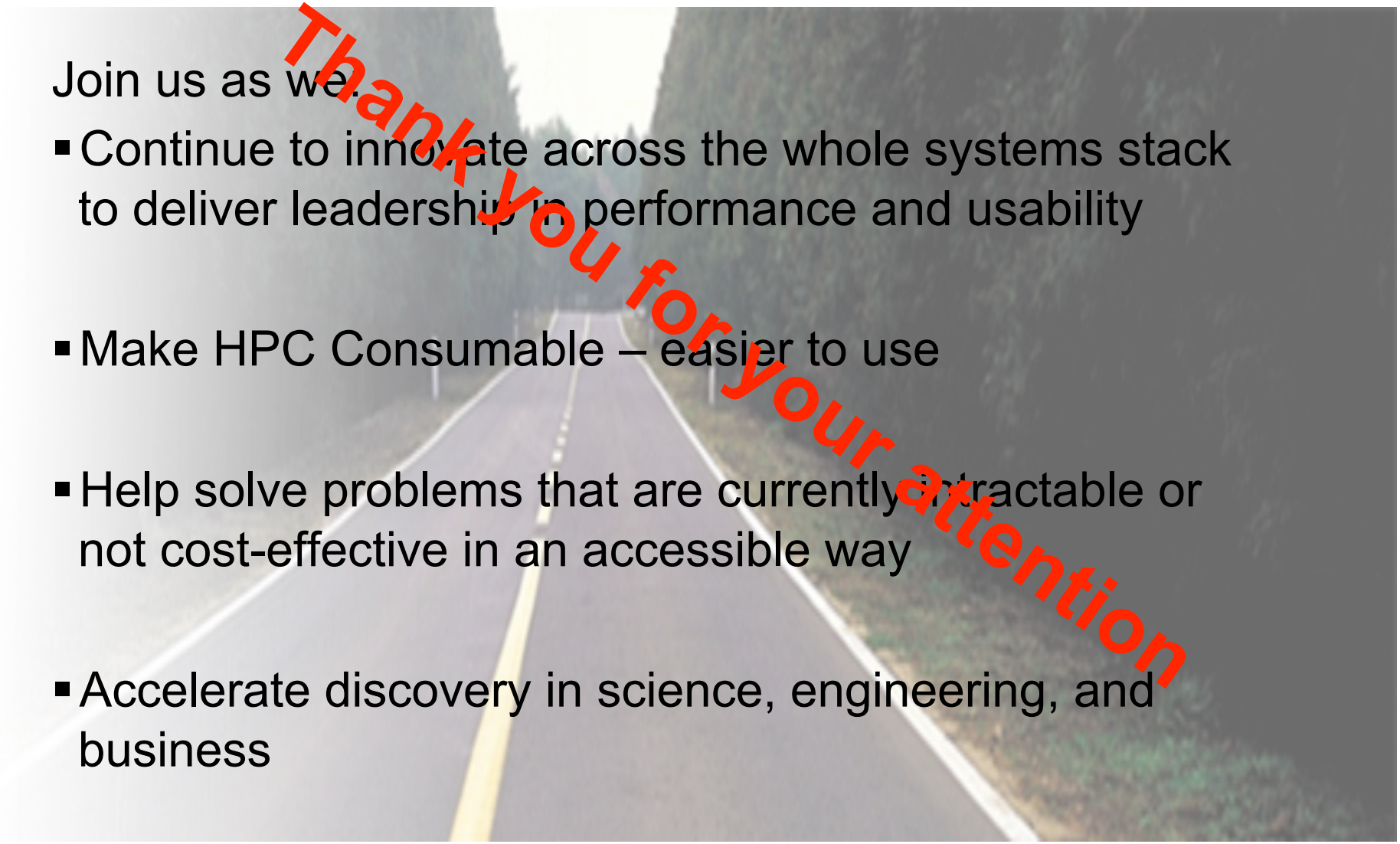

Join us as we:

- Continue to innovate across the whole systems stack to deliver leadership in performance and usability
- Make HPC Consumable – easier to use
- Help solve problems that are currently intractable or not cost-effective in an accessible way
- Accelerate discovery in science, engineering, and business