ISC High Performance
The HPC Event.

KAUST Activities in Extreme Computing

David Keyes, Applied Mathematics & Computational Science
Director, Extreme Computing Research Center (ECRC)
King Abdullah University of Science and Technology

جامعة الملك عبد الله
للعلوم والتقنية
King Abdullah
University of Science...
Discovery
Square
Economic Development
and Research Park
of Oman

Research Universities

FOR

DUMMIES®

2nd Edition

Survive conflicts of expectation— and deliver on dreams!

A Reference for the Rest of Us!®

Part I

KAUST's pillars, paradigms and strategies

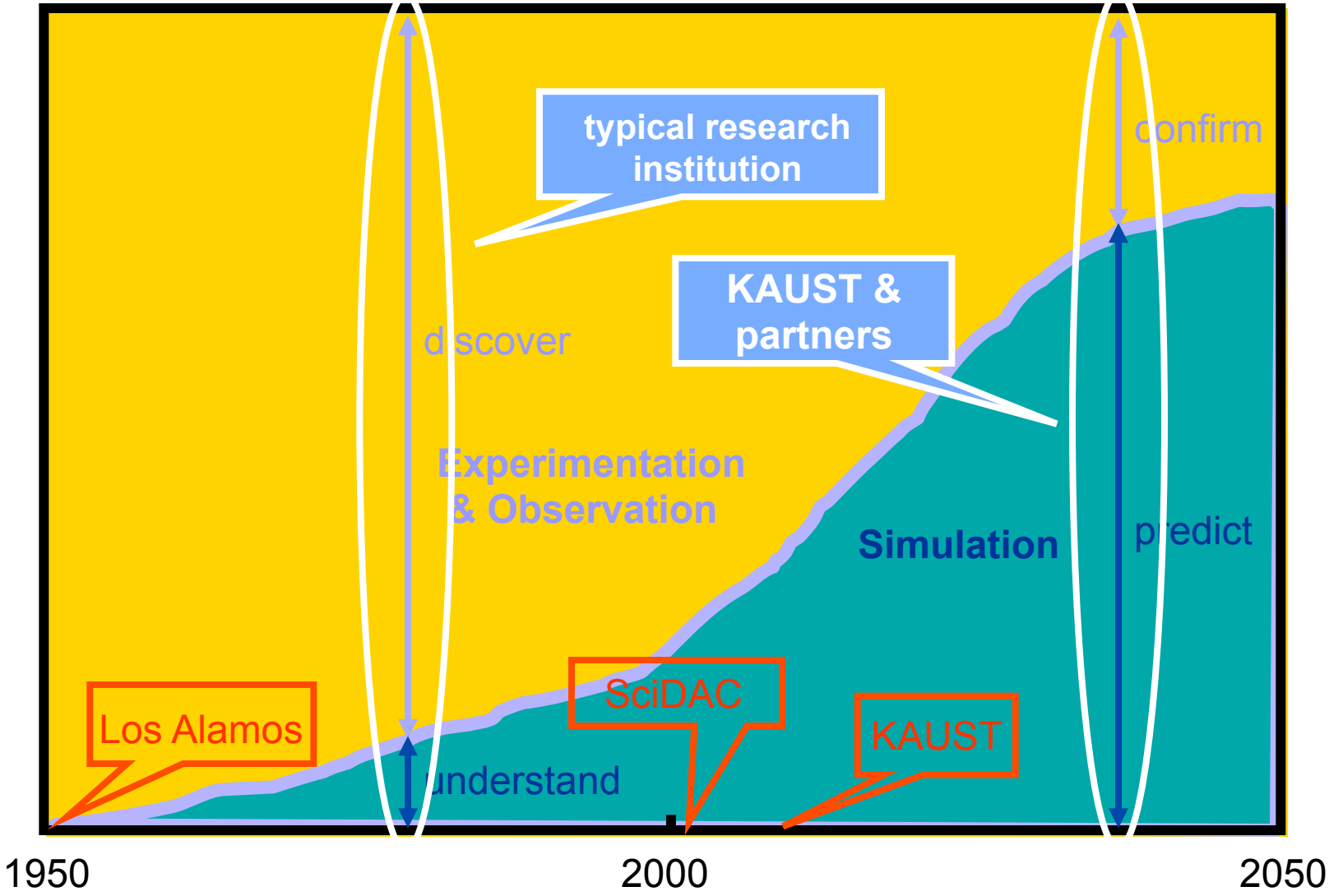
KAUST is a research institution with four sustainability "pillars":

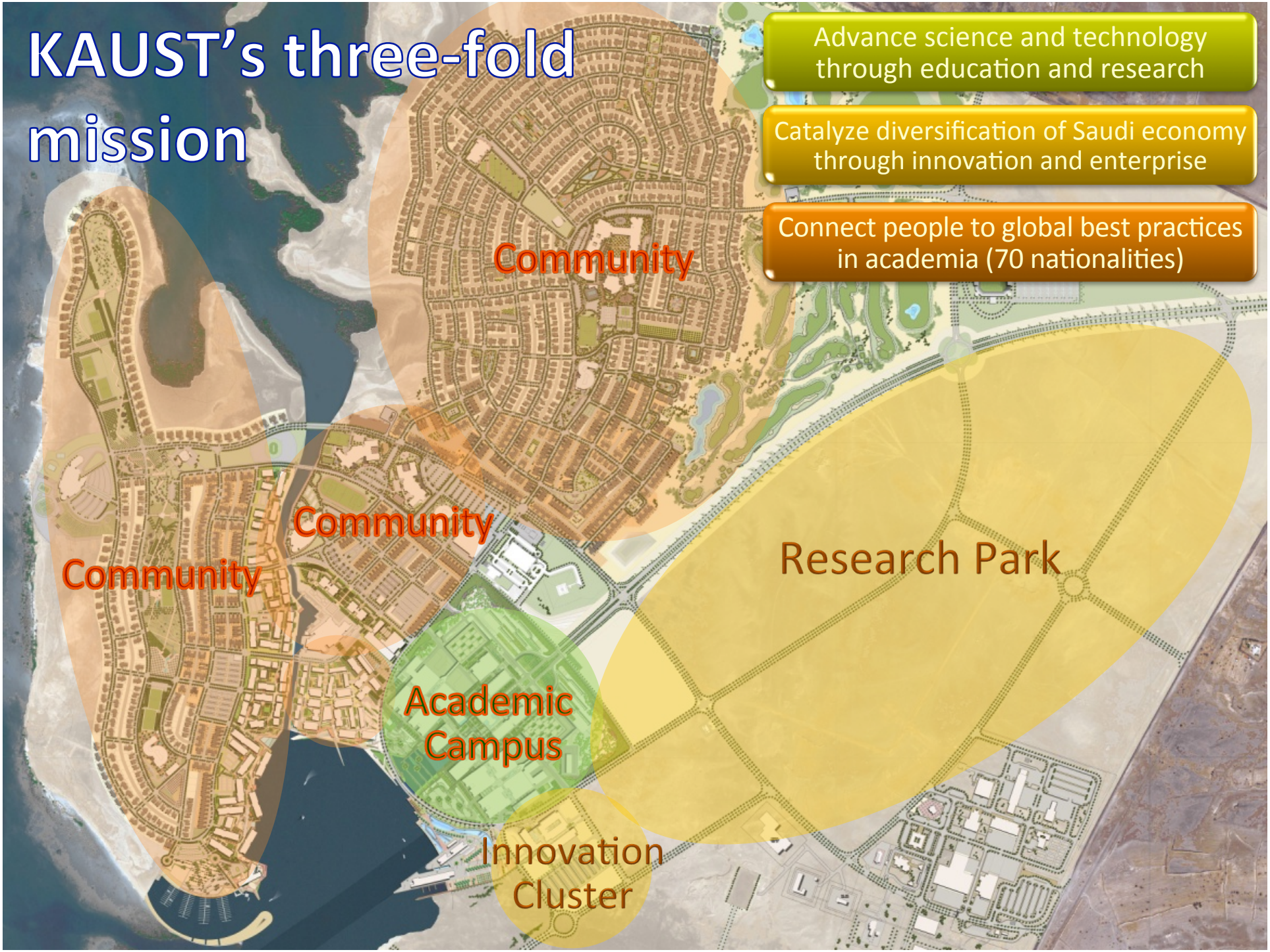
… and computational science as an "enabler"

… with four paradigms to employ

(many institutions are still firing on just two of the four cylinders)

Advance of the third paradigm




KAUST's three-fold mission
Advance science and technology through education and research
Catalyze diversification of Saudi economy through innovation and enterprise
Connect people to global best practices in academia (70 nationalities)
Community
Community
Community
Research Park
Academic Campus
Innovation Cluster

KAUST's overall strategy: leapfrog

KAUST faces two means to achieve its mission of

- Advancing science and technology
- Catalyzing economic diversification
- Connecting Saudi Arabia to best practices in research and academic culture

1. **Patiently follow the leaders**
   - Do what they do, long and well, *or*
2. **"Reinvent" the research university**
   - Emphasize what others may find less natural, being "trapped" in their success

KAUST's strategy #1: Multidisciplinarity

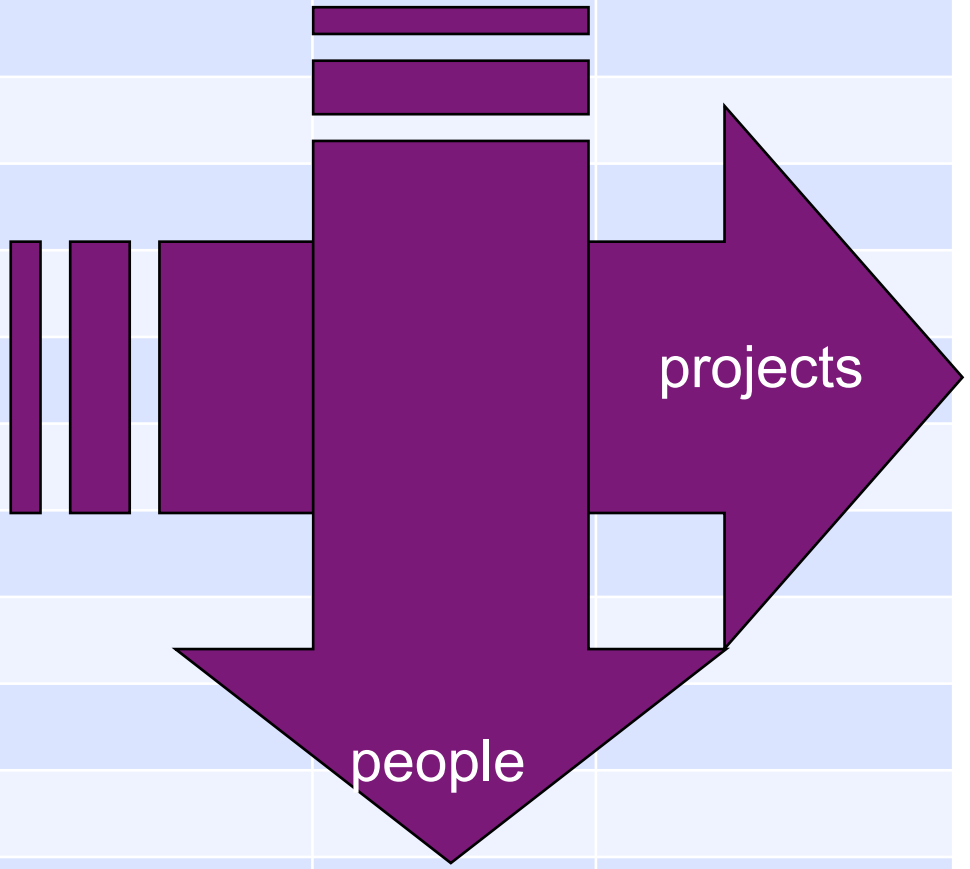
- KAUST is structured to capitalize on neglected ground between traditional disciplines
- Science and engineering are administered together as equals
- Mission-driven research centers draw expertise required from any academic unit, by adding independent resources
- Disciplinary territoriality is reduced
  - no student credit hour-based budgeting
  - faculty lines assigned to serve missions

KAUST's matrix structure, 2015

Divisions

Centers

	BESE	CEMSE	PSE
Catalysis			
Clean Combustion			
Membranes			
Plant Stress Genomics			
Red Sea Studies			
Solar Photovoltaics			
Upstream Petroleum			
Water Desalination & Reuse			
Computational Biosciences			
Extreme Computing			
Visual Computing			



KAUST's strategy #2: Big Sisters
degree program founding partners

Partner	Program
Stanford	Computer Sci
Stanford	Applied Math & Computational Sci
Berkeley	Mechanical Eng
Michigan	Electrical Eng
Texas	Earth Sci & Eng
Illinois	Environmental Sci & Eng
Woods Hole*	Marine Sci & Eng
Imperial College	Materials Sci & Eng
Cambridge	Biological Sci & Eng

* small partner

KAUST's strategy #2: Big Sisters

research program founding partners

Stanford

Texas A&M

Cornell

Oxford

Utrecht

KFUPM

NTU

KAUST's strategy #3:
Industry and Entrepreneurship

KAUST's strategy #3: Industry and Entrepreneurship

- **KAUST aims that regional industrial demand will drive much on-campus research**
- **Faculty, post-docs, students are encouraged and enabled to be entrepreneurs with**
  - **short courses**
  - **industrial partners in residence**
  - **seed funding**
  - **expert staffing for IP, fund raising, etc.**

KAUST's strategy #3: Industry and Entrepreneurship Student and staff start-ups

Acadox	**Touching Care**	**iDivers**	**Muse Tech**	**NOMADD**
Social Network	Healthcare	Marine and Recreational Diving	Arts and Entertainment	Renewable Energy
Nedal Murad, Mustafa Nabulsi, Mohammad Alhareeqi – Graduate Students	Rawad Shiek – Graduate Student	Michael Berumen - Faculty	Steven Cutchin - Staff	Georg Eitelhuber - Staff
Community-based system facilitating academic life	Software tool customized for Alzheimer patients and caregivers	First underwater full functionality tool for iPad and iPhone devices	A photo-real 3D immersive environment for museums	Cost effective and environmentally friendly cleaning devise for desert-based solar installations

4 of first 5 start-ups are in domain of information technology

KAUST's strategy #4: Facilities

Seven state-of-the-art core labs

- *Supercomputing*
- *Scientific visualization*
- Nanofabrication
- DNA sequencing
- Imaging and characterization
- Marine science
- Machine fabrication

KAUST's strategy #4: Facilities

CORNEA

SHAHEEN

Shaheen II

KAUST Supercomputing Lab

جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology

Shaheen II Specs

- 36 cabinets of Cray XC40 with Intel Haswell 2.3 Ghz with 16 cores
- 128 GB of RAM per node
- Number of nodes: 6192
- Number of cores: 198144
- Peak Performance: 7.3 PFlops/s
- LINPACK : 5.6 PFlops/s
- 2.8 MW at peak
- 17.4 PB of Parallel File System
- I/O throughput: over 500 GB/s
- Burst Buffer capacity: 1.5 TB
- Burst Buffer throughput: over 1.2 TB/s

Newly ranked:
#7 on HPL
#7 on HPCG

~2 GF/s/W

CSE 2009: The World's First CSE University

June 15, 2009

The King Abdullah University of Science and Technology, scheduled to welcome its first class of students in September, sponsored a reception in Miami on March 2, the first day of the SIAM Conference on Computational Science and Engineering. David Keyes and Omar Ghattas, involved in different ways in the new venture, hosted the reception and made informal presentations to the assembled crowd.

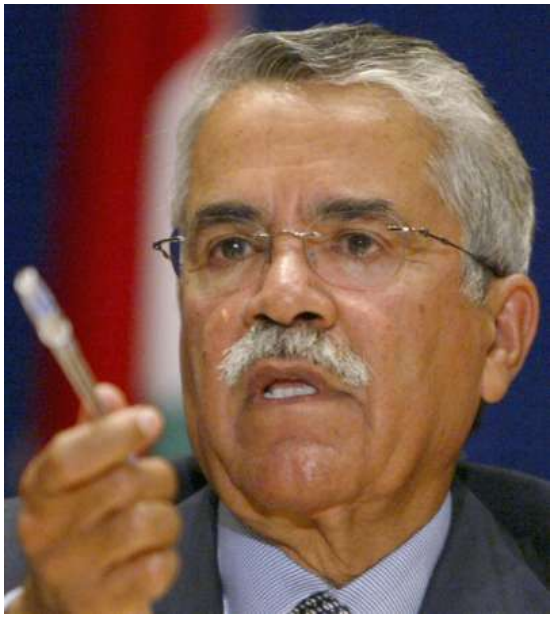
Most readers will know something of KAUST, which for the record is a graduate-only (master's and doctoral) university being constructed in Saudi Arabia, on the eastern edge of the Red Sea, not far from Jeddah. Keyes, the inaugural chair of KAUST's Mathematical and Computer Sciences and Engineering Division, offered examples of research areas of particular interest to Saudi Arabia and the region that will be emphasized; among them are geophysics, seismology, reservoir modeling, CO2 sequestration, photovoltaics, stress-tolerant agriculture, desalination, catalysis, and materials, along with the applied mathematics and computer science required to support them.

Sizeable recruitment ads for KAUST have appeared in many recent issues of *SIAM News*, often side by side with ads placed by partners of the new university, such as the

How we got here

The VISION

The EXECUTION



The DESIGN

KAUST in brief

- Language of instruction is English
- At maturity (ramping up over ten years), KAUST will have ~1,500 students (1/3 M.S. and 2/3 Ph.D.)
- At maturity, KAUST will have ~225 faculty members
- Full research community at KAUST will consist of ~1,500 people, in addition to the thesis students
- At maturity, the KAUST community will have 15,000 residents
- Holds one of the top few university endowments
- "Caltech-sized university on a Yale-sized endowment"

KAUST in brief

Graduate university governed by independent, self-perpetuating Trustees, operated off of an independently held endowment, with Western-style charter

Open to men and women from all over the world

Organized as a matrix of academic divisions and research centers

Globally connected at creation through KAUST-funded partnerships

Engaged in collaborative research with the private sector to advance economic development

Occupying a state-of-the-art, LEED-certified, environmentally responsible campus

2015 Leiden size-independent rankings

http://www.leidenranking.com

THOMSON REUTERS

Rank	University	Country
1	MIT	
2	Harvard Univ	
3	Stanford Univ	
4	Univ Calif - Berkeley	
5	Princeton Univ	
6	Caltech	
7	Univ Calif - Santa Barbara	
8	Univ Calif - San Francisco	
9	Rice Univ	
10	Weizmann Inst Sci	
11	London Sch Hyg & Trop Med	
12	Univ Calif - Santa Cruz	
13	Yale Univ	
14	Univ Texas - Southwestern Med Ctr	
15	Ecole Polytech Fed Lausanne	
16	Univ Calif - San Diego	
17	Univ Oxford	
18	Univ Chicago	
19	Columbia Univ	
20	Univ Calif - Los Angeles	
21	Northwestern Univ	
22	Univ Colorado - Boulder	
23	Univ Cambridge	
24	Univ Penn	
25	ETH Zurich	
26	Univ Massachusetts Med Sch	
27	Univ Washington - Seattle	
28	Cornell Univ	
29	Washington Univ - St Louis	
30	NYU	
31	Duke Univ	
32	Univ Coll London	
33	Imperial Coll London	
34	Univ Exeter	
35	King's Coll London	
36	Johns Hopkins Univ	
37	Icahn Sch Med - Mt Sinai	
38	Boston Coll	
39	Univ N Carolina - Chapel Hill	
40	Univ Basel	
41	Univ Lausanne	
42	Boston Univ	
43	Univ Bristol	
44	Univ Calif - Riverside	
45	Univ St Andrews	
46	Univ Calif - Irvine	
47	Univ Texas - Austin	
48	Univ Michigan	
49	Georgia Inst Technol	
50	Univ Texas Hlth Sci Ctr - Houston	
51	Vanderbilt Univ	
52	Leiden Univ	
53	Univ Southern Calif	
54	Univ Dundee	
55	Univ Aberdeen	
56	Univ Wisconsin - Madison	
57	Emory Univ	
58	Univ Maryland - College Park	
59	Dartmouth Coll	
60	Utrecht Univ	
61	Univ Geneva	
62	Univ Massachusetts Amherst	
63	Univ Edinburgh	
64	VU Univ Amsterdam	
65	Carnegie Mellon Univ	
66	École Polytech	
67	Univ Illinois - Urbana-Champaign	
68	Univ Amsterdam	
69	Univ York	
70	Tufts Univ	
71	Katholieke Univ Leuven	
72	Paris Descartes Univ	
73	Yeshiva Univ	
74	Univ Calif - Davis	
75	King Abdullah Univ Sci & Technol	

Part II
Extreme Computing

Roadmap for ECRC research

INTERNATIONAL EXASCALE SOFTWARE PROJECT ROADMAP 1.0

Jack Dongarra, Pete Beckman, Terry Moore, Patrick Aerts, Giovanni Aloisio, Jean-Claude Andre, David Barkai, Jean-Yves Berthou, Taisuke Boku, Bertrand Braunschweig, Franck Cappello, Barbara Chapman, Xuebin Chi

Alok Choudhary, Sudip Dosanjh, Thom Dunning, Sandro Fiore, Al Geist, Bill Gropp, Robert Harrison, Mark Hereld, Michael Heroux, Adolfy Hoisie, Koh Hotta, Yutaka Ishikawa, Fred Johnson

Sanjay Kale, David Keyes, Jesus Labarta, Alain Lichnewsky, Thomas Lippert, Bob Lucas, Barney Maccabe, Satoshi Matsuoka, Paul Messina, Peter Michielse, Bernd Mohr

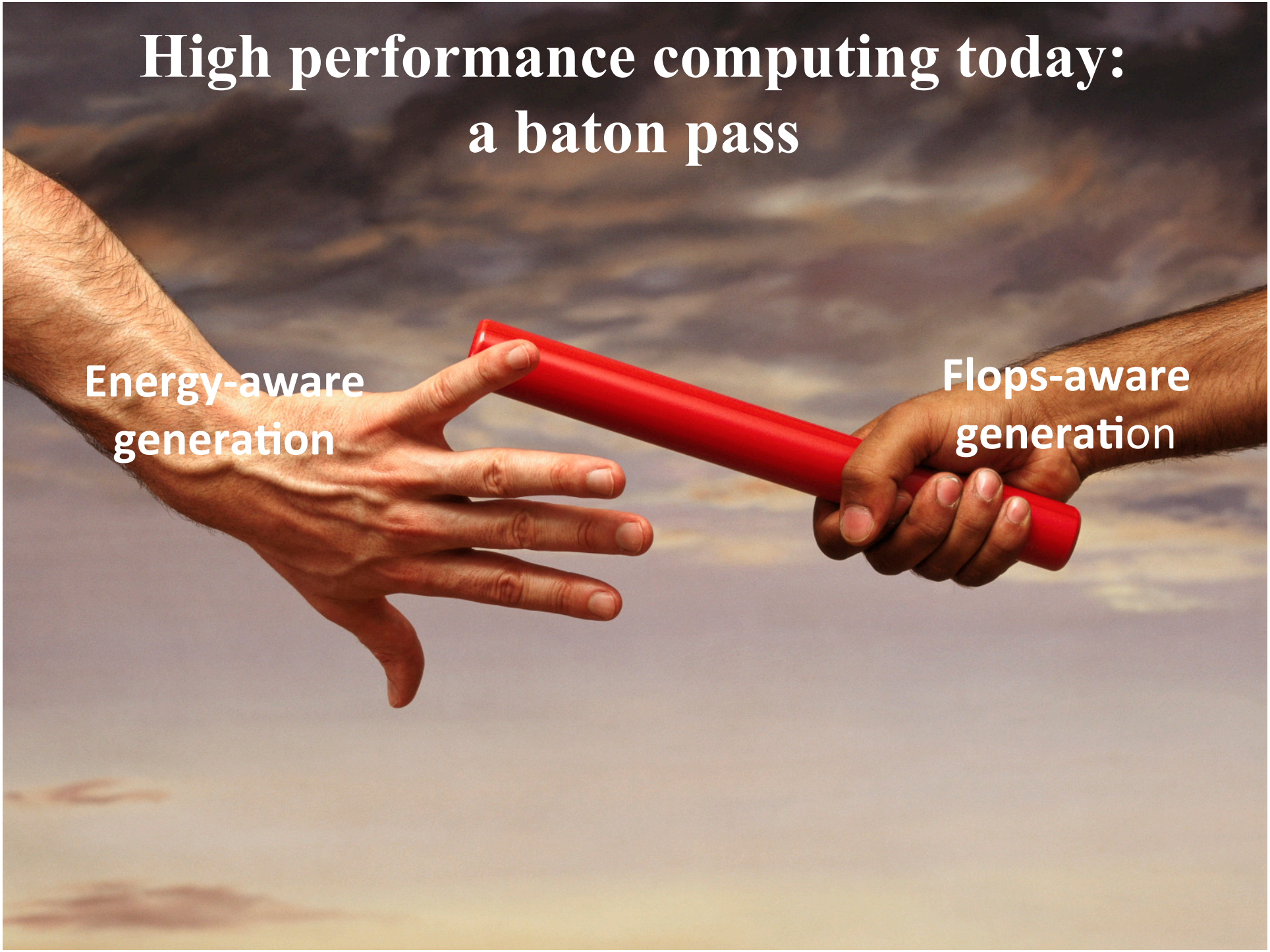
Matthias Mueller, Wolfgang Nagel, Hiroshi Nakashima, Michael E. Papka, Dan Reed, Mitsuhisa Sato, Ed Seidel, John Shalf, David Skinner, Marc Snir, Thomas Sterling, Rick Stevens, Fred Streitz

Bob Sugar, Shinji Sumimoto, William Tang, John Taylor, Rajeev Thakur, Anne Trefethen, Mateo Valero, Aad van der Steen, Jeffrey Vetter, Peg Williams, Robert Wisniewski, Kathy Yelick

SPONSORS

The International Exascale Software Roadmap, J. Dongarra, P. Beckman, et al., *International Journal of High Performance Computer Applications* **25**(1), 2011, ISSN 1094-3420.

High performance computing today: a baton pass



ECRC current students

Ali
Lebanon

Amani
Saudi

Chengbin
China

Dalal
Jordan

Gustavo
Mexico

Huda
Jordan

Lulu
China

Mohammed
Saudi

Mustafa
Syria

Noha
Saudi

Tareq
Jordan

Wajih
Lebanon

ECRC student or post-doc alumni

Ahmad
UTenn

Aron
USArmy ERDC

Enas
OSU

Jennifer
UManchester

Kai
SINTEF

Xiangliang
KAUST

Yuxin
(tbd)

Other faces of the ECRC

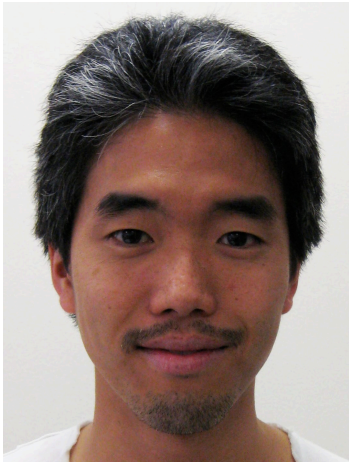
George Turkiyyah
Research Scientist

Hatem Ltaief
Research Scientist

Valerio Pascucci
Visiting Professor

Stefano Zampini
Research Scientist

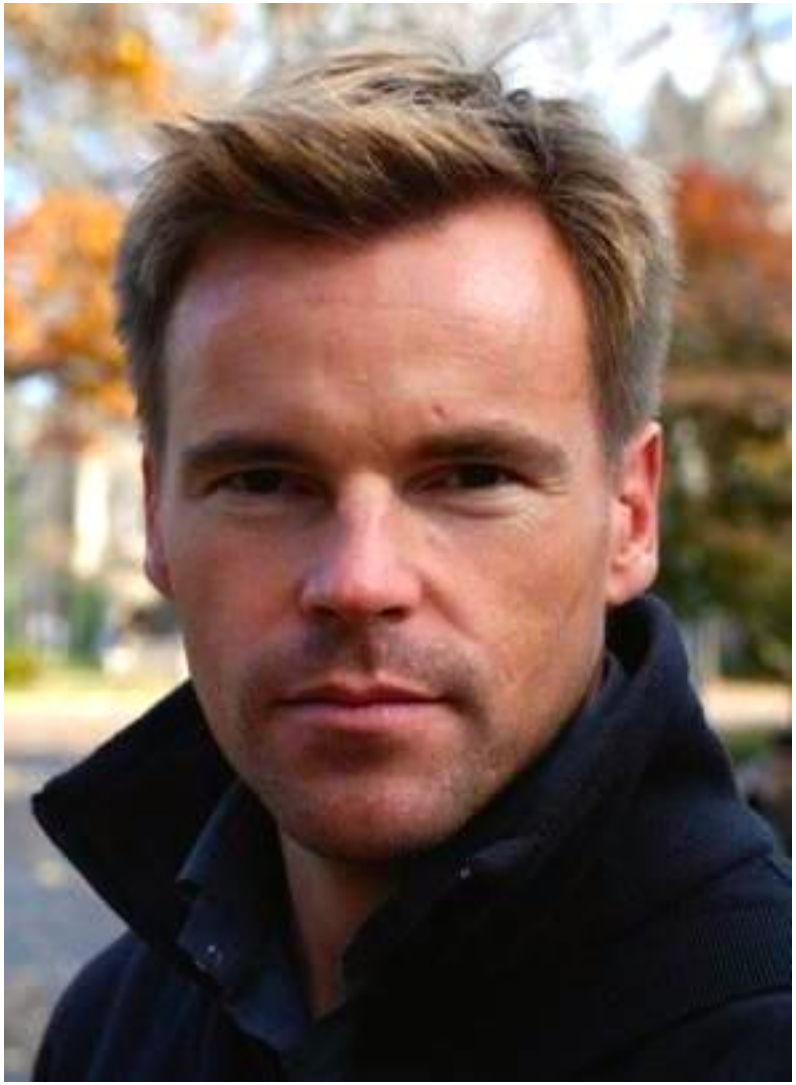
Alex Litvinenko
Research Scientist



Rio Yokota
Visiting Professor

ECRC's newest faculty appointees

- Daniel Peter
- PhD, ETH, 2008
- Numerical methods for seismic wave propagation
- Applications of high performance computing
- Architect of SPECFEM3D_GLOBE



ECRC's newest faculty appointees

- Matteo Parsani
- PhD, Frije Universiteit Brussel, 2010
- Numerical methods for compressible and reacting flows
- Applications of high performance computing
- Co-designer of NASA's FUN3D design code

KAUST's PETSc developers

PETSc Team

- Home
- Download
- Features
- Documentation
- Applications/Publications
- Miscellaneous
  - PETSc Team
  - Mailing Lists
  - Acknowledgements
  - Funding
  - Threads and PETSc
- External Software
- Developers Site

Please do not email individual PETSc authors. E-mail to petsc-maint@mcs.anl.gov is automatically distributed to the authors, so our response time using this address will be fastest.

Current Active Developers (August 2014)

Shrirang Abhyankar

Mark Adams

Satish Balay

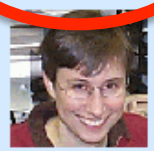
Jed Brown

Lisandro Dalcin

Tobin Isaac

Dmitry Karpeev

Matthew Knepley


Lois Curfman

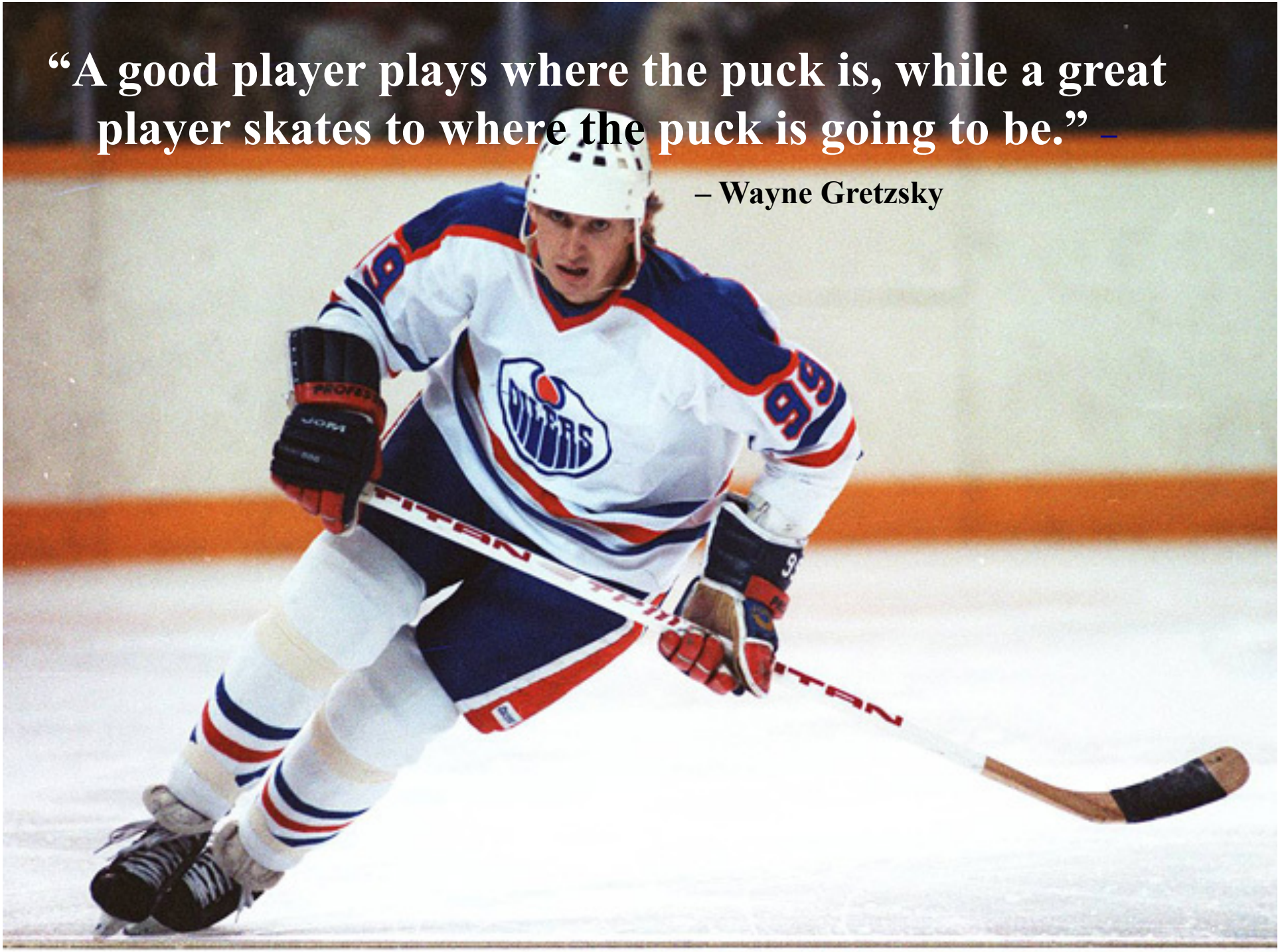
Karl Rupp

Jason Sarich

Barry Smith

Stefano Zampini

Hong Zhang


"A good player plays where the puck is, while a great player skates to where the puck is going to be." –
– Wayne Gretzsky

ECRC aspiration

- **To paraphrase Gretzsky:**

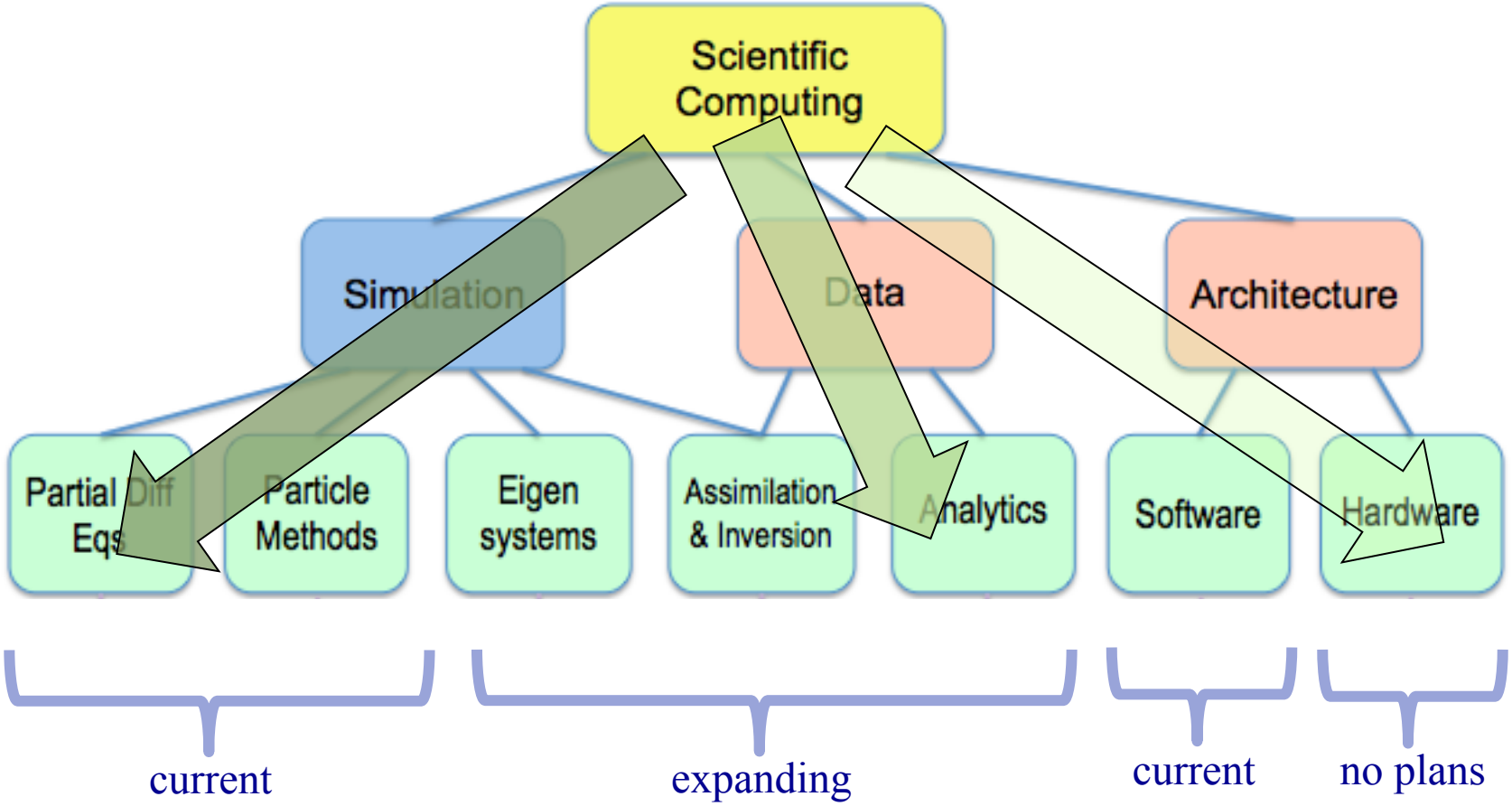
  "Algorithms for where architectures are going to be"

Such algorithms may *or may not* be the best today; however, hardware trends can be extrapolated to their sweet spots.

ECRC's twin deliverables

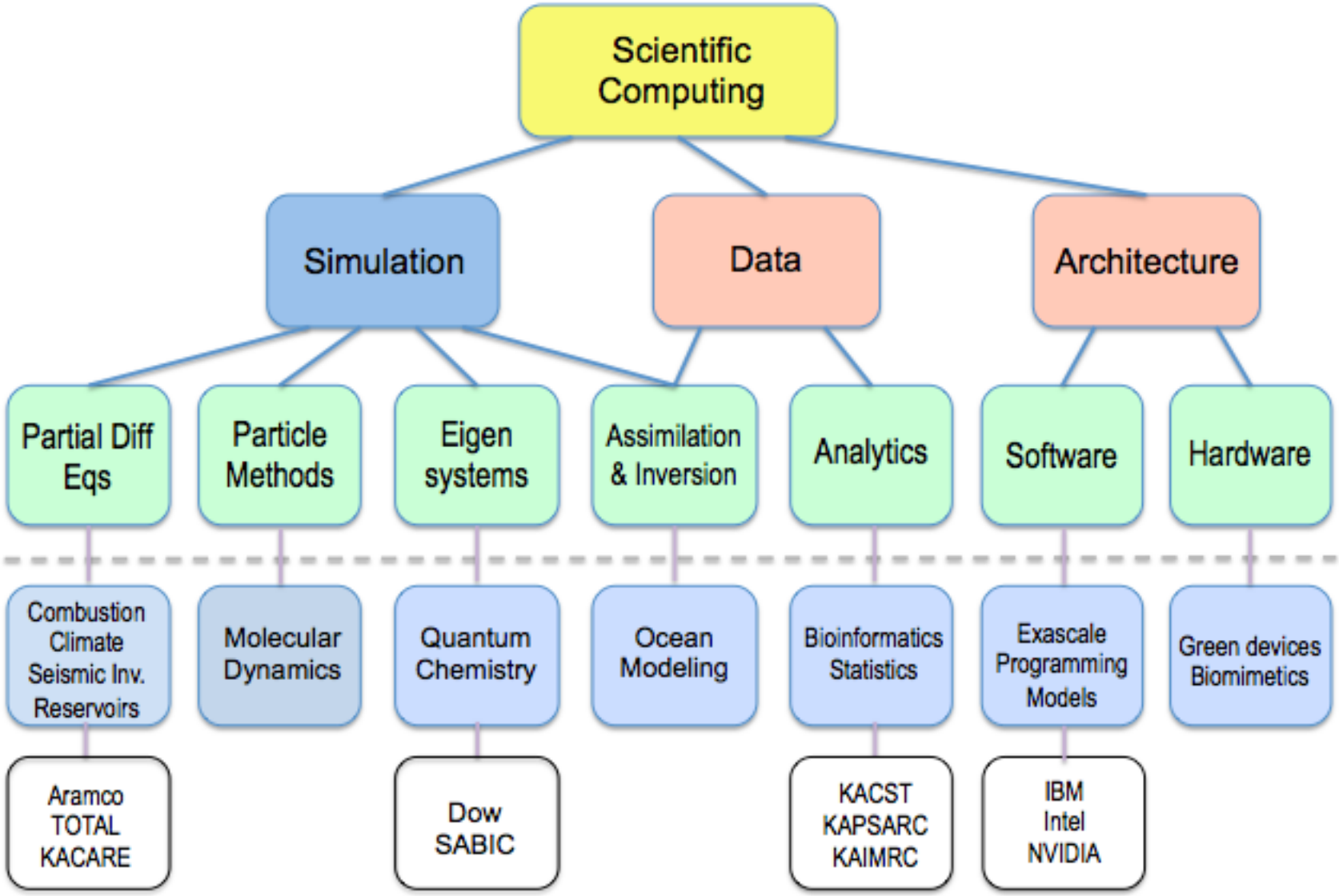
- **Develop and demonstrate algorithms for scientific simulation and data analytics at emerging architectural scales**
  - **most of today's scientific libraries are designed for a different environment (BSP) and need to be evolved**
- **Raise the impact and increase the reach of scientific simulation and data analytics at KAUST**
  - **pursuit of performance requires specialization complementary to expertise of computational scientists and engineers**

Vision for extreme computing at KAUST



Topical foci of the ECRC relative to the spectrum of scientific computing at KAUST today

Vision for extreme computing at KAUST



Required software enabling technologies

Model-related

- Geometric modelers
- Meshers
- Discretizers
- Partitioners
- Solvers / integrators
- Adaptivity systems
- Random no. generators
- Subgridscale physics
- Uncertainty quantification
- Dynamic load balancing
- Graphs and combinatorial algs.
- Compression

Development-related

- Configuration systems
- Source-to-source translators
- Compilers
- Simulators
- Messaging systems
- Debuggers
- Profilers

Production-related

- Dynamic resource management
- Dynamic performance optimization
- Authenticators
- I/O systems
- Visualization systems
- Workflow controllers
- Frameworks
- Data miners
- Fault monitoring, reporting, and recovery

High-end computers come with little of this stuff. Most has to be contributed by the user community

Relation to KAUST's economic mission

- **Enable advances through simulation for the KSA's largest industry today:**
  - **seismic imaging for petroleum discovery**
  - **reservoir simulation for petroleum production**
  - **computational chemistry for downstream petroleum processing**
- **Attract an important industry the KSA does not possess today:**
  - **information technology**

NVIDIA GPU RESEARCH CENTER

intel Intel Parallel Computing Centers

CRAY THE SUPERCOMPUTER COMPANY

CENTER OF EXCELLENCE

Collaborations within KAUST

- **Obvious center collaborations:**
  - **Combustion, Catalysis, Red Sea**
- **Possible center collaborations:**
  - **Water Desalination, Membranes, Computational Biosciences, Solar & Renewables**
- **Core laboratories:**
  - **Supercomputing Laboratory**
  - **Visualization Laboratory**

Collaborations within the KSA

- **Agencies/ministries:**
  - **KACARE, KACST, KAIMRC, KAPSARC**
- **Universities:**
  - **KFUPM, UQU**
- **Companies:**
  - **Aramco, SABIC**

Collaborations outside the KSA

- Computational science and computer science programs at national laboratories of the U.S. DOE and European PRACE
- IT vendors:
  - Cray, IBM, Intel, NVIDIA, and others
- IT customers:
  - Total and others
- EU Horizon2020 institutions
- Other international universities

Algorithmic agenda

- New formulations with
  - greater arithmetic intensity (flops per byte moved into and out of registers and upper cache)
    - including assured accuracy with (adaptively) less floating-point precision
  - reduced synchronization and communication
    - less frequent *and/or* less global
  - greater SIMD-style thread concurrency for accelerators
  - algorithmic resilience to various types of faults
- Quantification of trades between limited resources
- *Plus* all of the exciting analytical agendas that exascale is meant to exploit
  - "post-forward" problems: optimization, data assimilation, parameter inversion, uncertainty quantification, etc.

Optimal hierarchical algorithms

- **At large scale, one must start with algorithms with optimal asymptotic scaling,** $O(N \log^p N)$
- **Some optimal hierarchical algorithms**
  - **Fast Fourier Transform (1960's)**
  - **Multigrid (1970's)**
  - **Fast Multipole (1980's)**
  - **Sparse Grids (1990's)**
  - **$\mathcal{H}$ matrices (2000's)**

"With great computational power comes great algorithmic responsibility." – Longfei Gao

Examples being developed at the Extreme Computing Research Center at KAUST

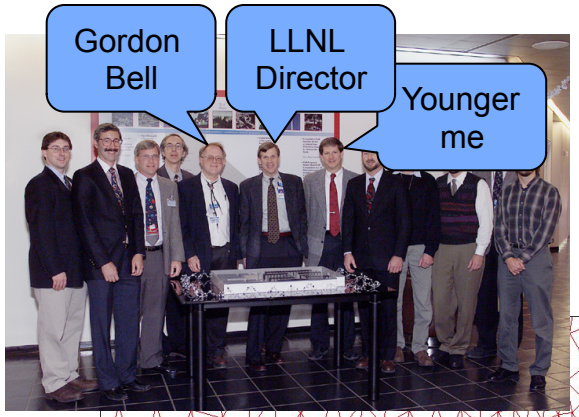
- **ACR, a new spin on 45-year-old cyclic reduction that recursively uses $\mathcal{H}$ matrices on Schur complements to reduce $O(N^2)$ complexity to $O(N \log^2 N)$**
- **FMM, a 30-year-old $O(N)$ solver for potential problems with good asymptotics but a bad constant when used at high precision, used in low precision as a FEM preconditioner**
- **QDWH-SVD, a 2-year-old SVD algorithm that performs more flops but generates essentially arbitrary amounts of dynamically schedulable concurrency, and beats state-of-the-art on GPUs**
- **MWD, a multicore wavefront diamond-tiling stencil evaluation library that reduces memory bandwidth pressure on multicore processors**
- **BDDC, a preconditioner well suited for high-contrast elliptic problems that trades lots of local flops for low iteration count, now in PETSc**
- **MSPIN, a new nonlinear preconditioner that replaces most of the global synchronizations of Newton iteration with local problems**

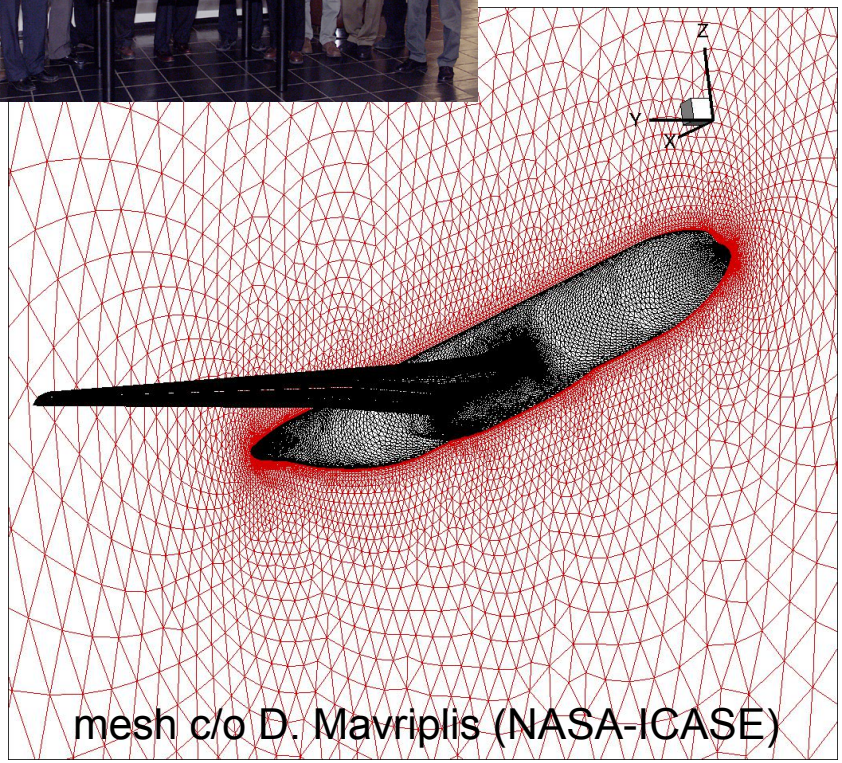
Three thumbnails of ECRC research

- **Collaboration with Intel on aerodynamics modeling**
- **Collaboration with *Observatoire de Paris* on adaptive optics for world's largest telescope**
- **Internal algorithmic research on "algebraic fast multipole"**

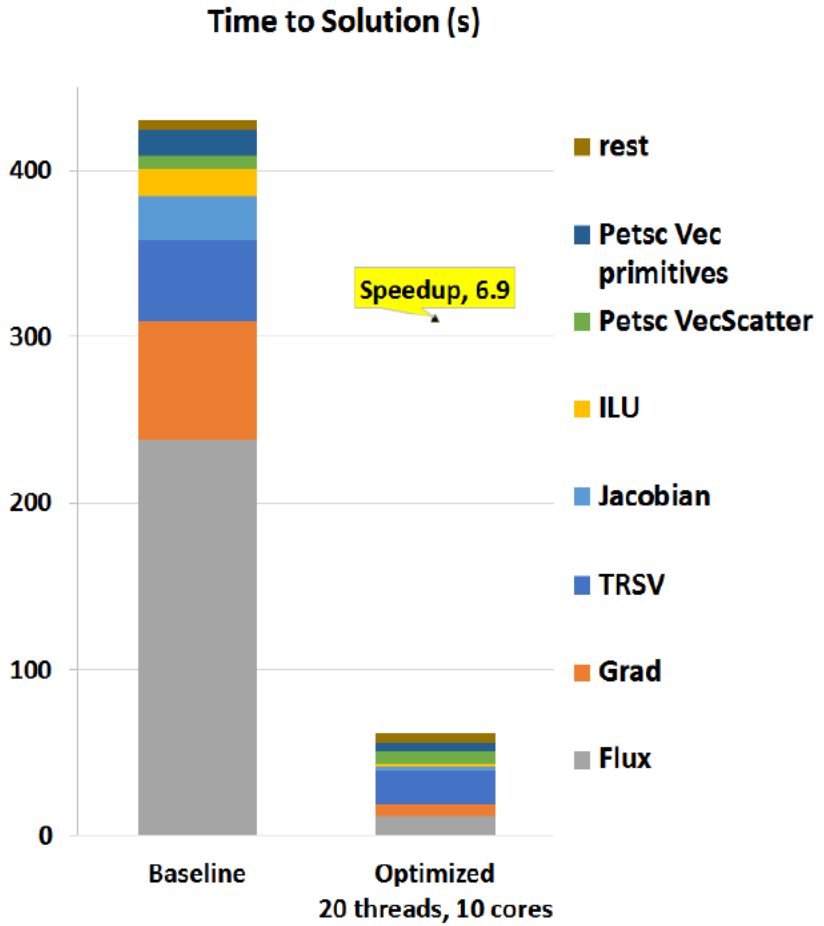
Computational aerodynamics

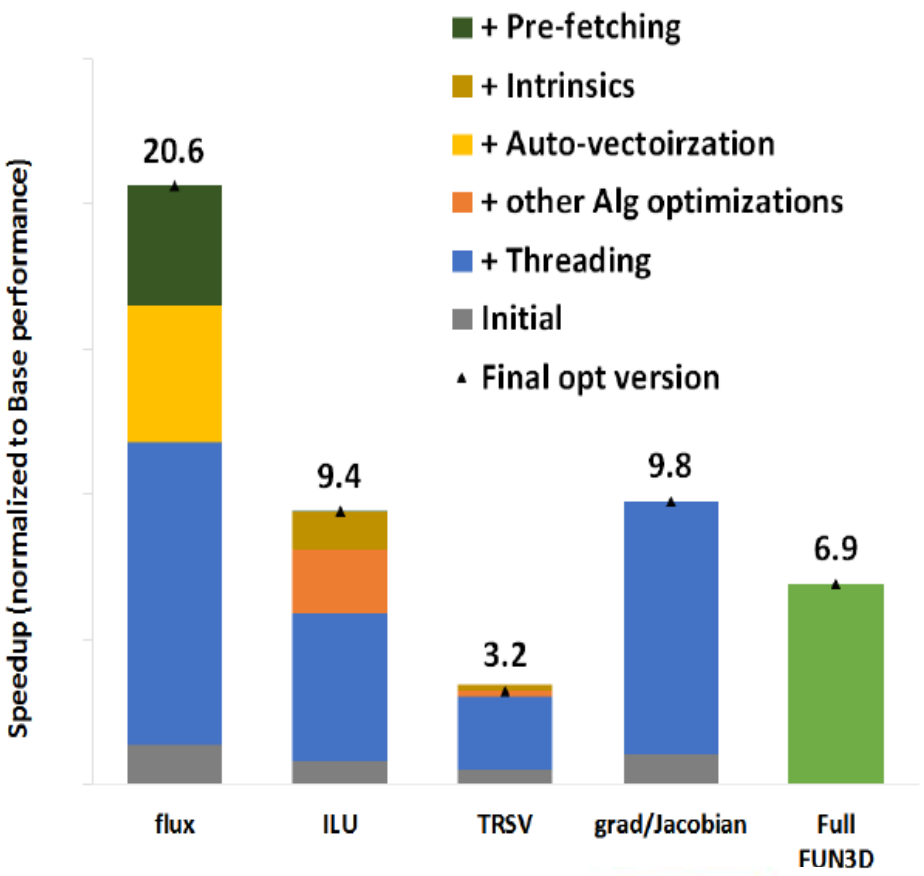
- **Our PETSc-FUN3D won an ACM Gordon Bell Prize in 1999 for distributed memory scaling of a fully implicit unstructured grid NASA external aircraft flow**
- **With Intel-Bangalore, we are porting this implicit unstructured grid code to Intel many-core chips for strong shared-memory scaling within a single compute node**





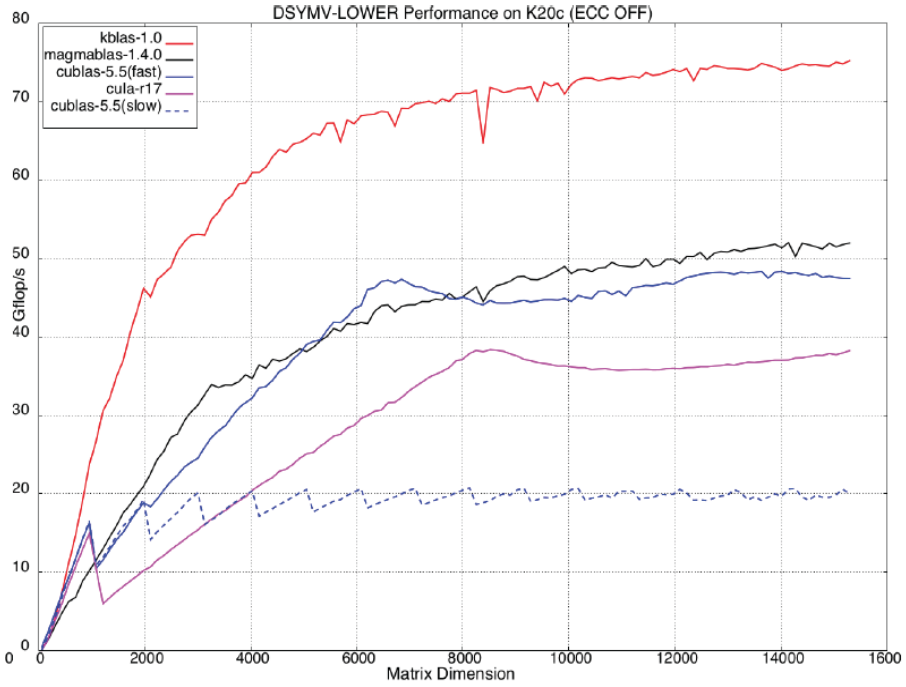
PETSc-FUN3D on Intel "Ivy Town"

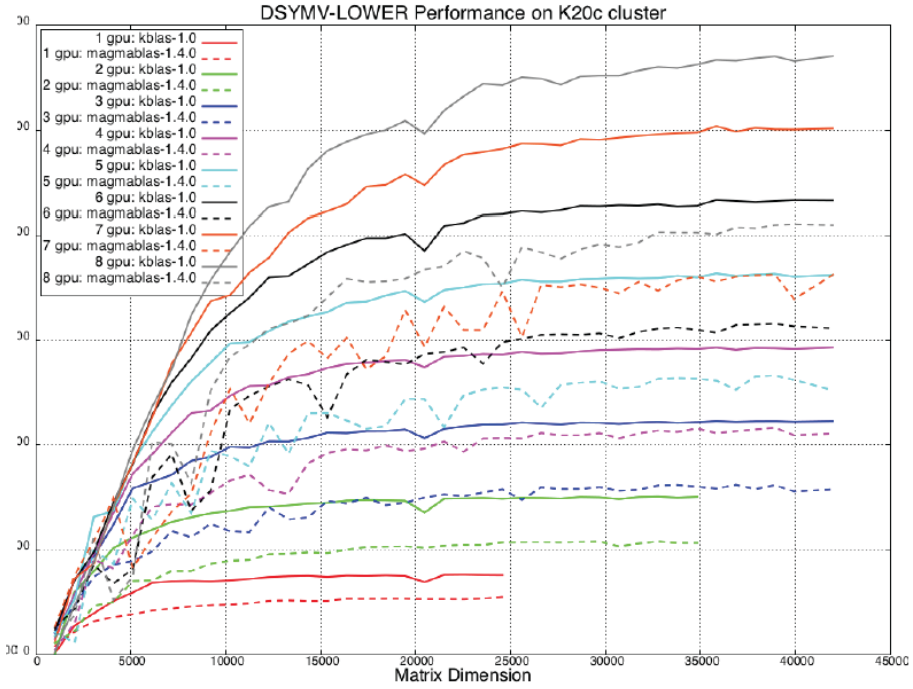




c/o A. Deshpande (Intel), submitted to SC'14

KAUST's software in NVIDIA's CUBLAS

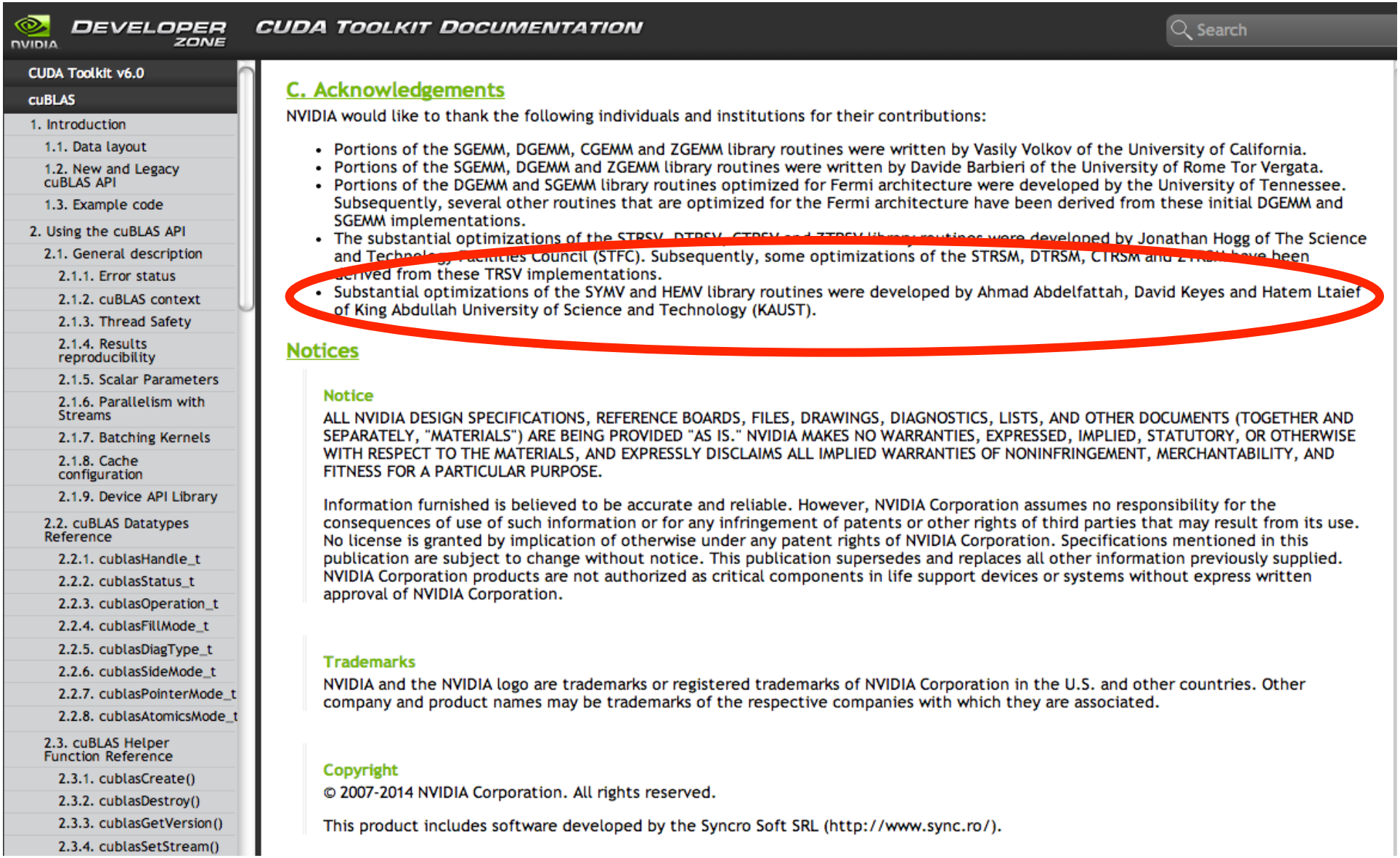




- **Highly optimized GEMV/SYMV kernels**
- **NVIDIA has adopted for its CUBLAS 6.0 library**

c/o Ahmad Abdelfattah (KAUST)

“KAUST inside”



NVIDIA DEVELOPER ZONE CUDA TOOLKIT DOCUMENTATION

Search

CUDA Toolkit v6.0

cuBLAS

1. Introduction
   - 1.1. Data layout
   - 1.2. New and Legacy cuBLAS API
   - 1.3. Example code
2. Using the cuBLAS API
   - 2.1. General description
     - 2.1.1. Error status
     - 2.1.2. cuBLAS context
     - 2.1.3. Thread Safety
     - 2.1.4. Results reproducibility
     - 2.1.5. Scalar Parameters
     - 2.1.6. Parallelism with Streams
     - 2.1.7. Batching Kernels
     - 2.1.8. Cache configuration
     - 2.1.9. Device API Library
   - 2.2. cuBLAS Datatypes Reference
     - 2.2.1. cublasHandle_t
     - 2.2.2. cublasStatus_t
     - 2.2.3. cublasOperation_t
     - 2.2.4. cublasFillMode_t
     - 2.2.5. cublasDiagType_t
     - 2.2.6. cublasSideMode_t
     - 2.2.7. cublasPointerMode_t
     - 2.2.8. cublasAtomicsMode_t
   - 2.3. cuBLAS Helper Function Reference
     - 2.3.1. cublasCreate()
     - 2.3.2. cublasDestroy()
     - 2.3.3. cublasGetVersion()
     - 2.3.4. cublasSetStream()

C. Acknowledgements

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- Portions of the SGEMM, DGEMM, CGEMM and ZGEMM library routines were written by Vasily Volkov of the University of California.
- Portions of the SGEMM, DGEMM and ZGEMM library routines were written by Davide Barbieri of the University of Rome Tor Vergata.
- Portions of the DGEMM and SGEMM library routines optimized for Fermi architecture were developed by the University of Tennessee. Subsequently, several other routines that are optimized for the Fermi architecture have been derived from these initial DGEMM and SGEMM implementations.
- The substantial optimizations of the STRSV, DTRSV, CTRSV and ZTRSV library routines were developed by Jonathan Hogg of The Science and Technology Facilities Council (STFC). Subsequently, some optimizations of the STRSM, DTRSM, CTRSM and ZTRSM have been derived from these TRSV implementations.
- Substantial optimizations of the SYMV and HEMV library routines were developed by Ahmad Abdelfattah, David Keyes and Hatem Ltaief of King Abdullah University of Science and Technology (KAUST).

Notices

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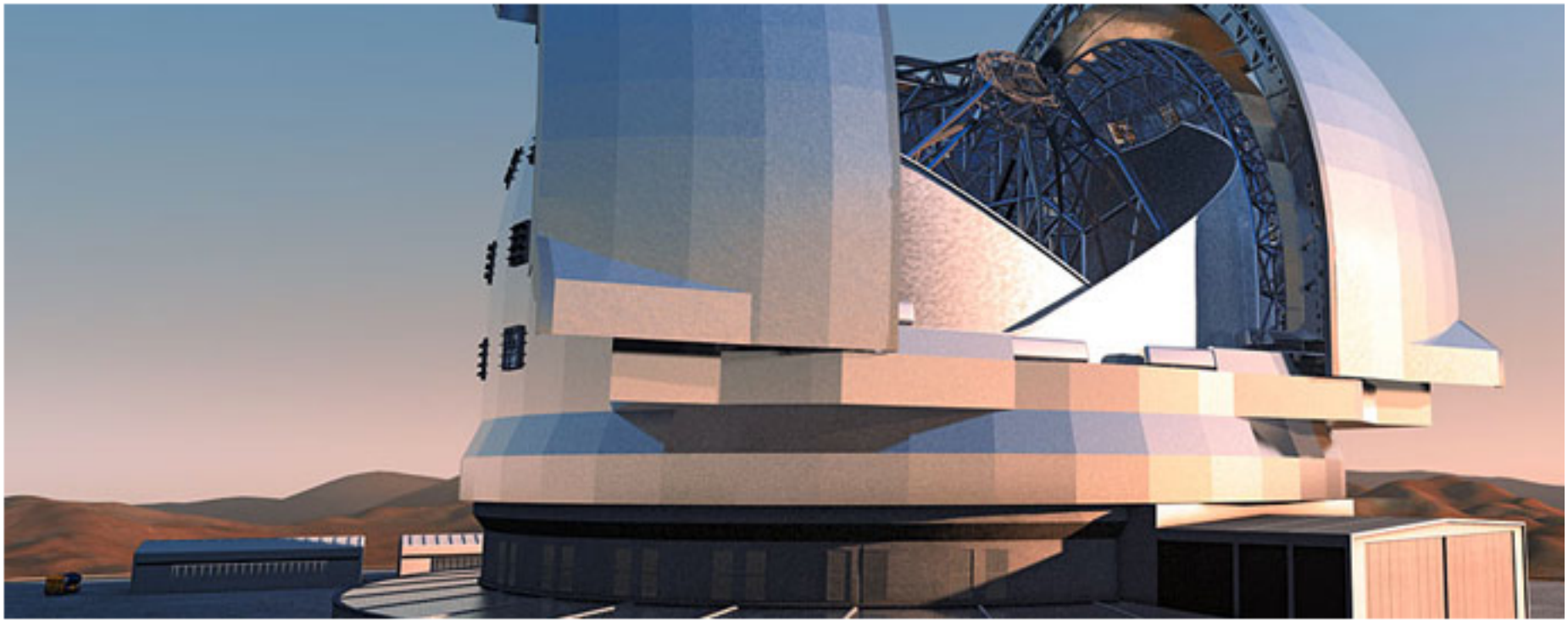
KAUST in European telescope (ELT)

The European Extremely Large Telescope

The world's biggest eye on the sky



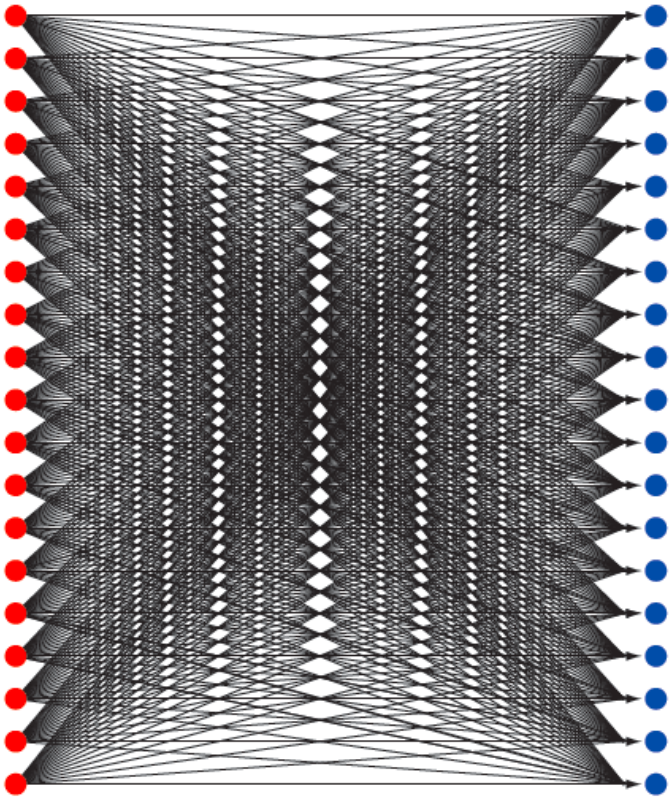
© ESO, https://www.eso.org/sci/facilities/develop/ao/ao_modes.html

c/o Ahmad Abdelfattah & Ali Charara (KAUST), SC'14

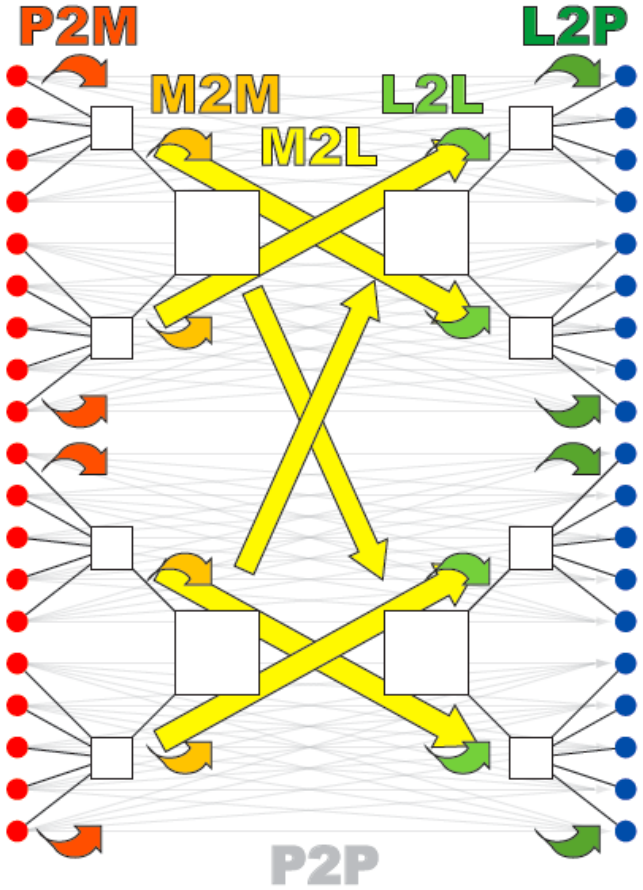
"Fast Multipole inside"

- **Fast Multipole is an optimal algorithm for a very frequently used specialized kernel in computational science (the "potential solve")**
- **Fast Multipole, which has led to Gordon Bell prizes in astrophysics, molecular dynamics, materials science, arterial dynamics, etc. has been highly optimized by KAUST Research Scientist Rio Yokota in "ExaFMM"**
  - **Can we leverage its excellent architectural properties for more general operators in applied science?**

Fast Multipole communication schema



(a) Direct method

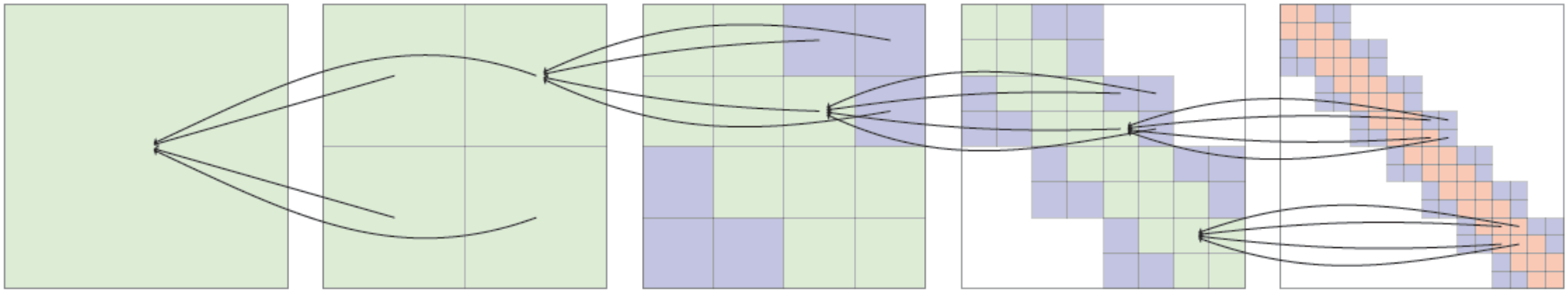


(b) Fast Multipole Method

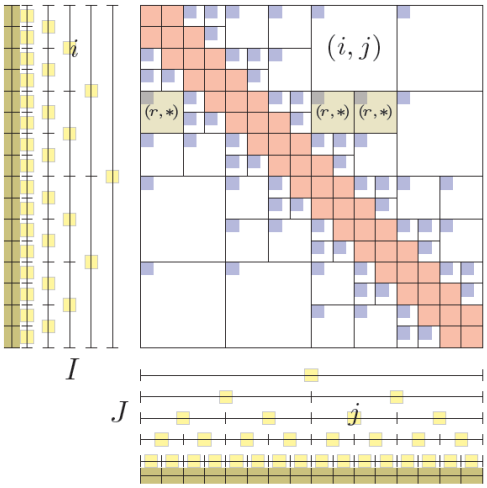
c/o R. Yokota, KAUST, *et al.*

"Algebraic Fast Multipole" (AFM)

- We have cast general matrix operations (add, multiply, invert, etc.) in terms of the fast multipole recursive "tree-based" data structure



- We first significantly compress the matrix, saving storage and operations
  - May offer breakthrough in application performance



c/o Wajih Boukaram (KAUST)

Part III
Large-scale Simulation at KAUST

Model for ECRC enablements

Mission: enable scientists and engineers to take advantage of petascale hardware by overcoming the scalability bottlenecks of traditional solvers, and assist users to move beyond one-off "forward" simulations to inversion, optimization, sensitivity, UQ, validation ($32M/10 years, 2001-11, PI: D. Keyes)

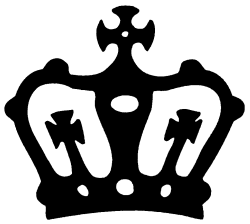
Argonne NATIONAL LABORATORY

Lawrence Livermore National Laboratory

TOPS

Towards Optimal Petascale Simulations

Sandia National Laboratories



Columbia University

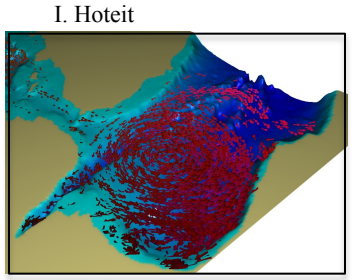
University of Colorado

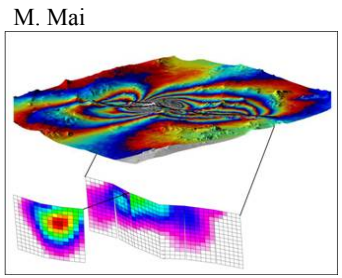
Berkeley
University of California

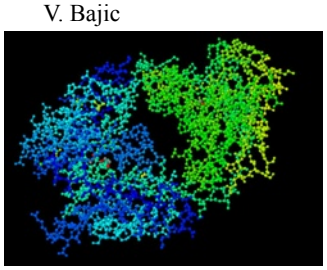
University of Texas

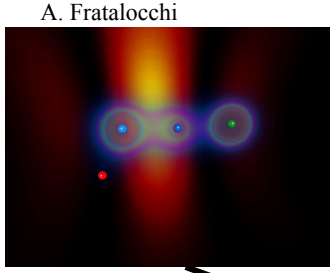
University of California at San Diego

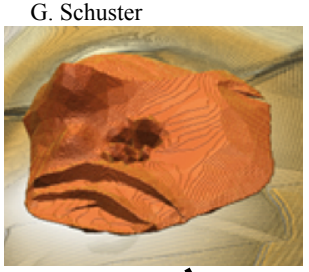
SciDAC-like model for software investments

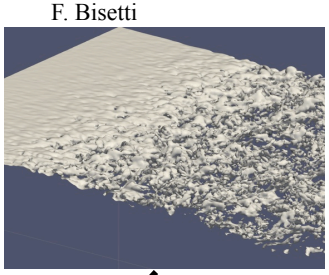


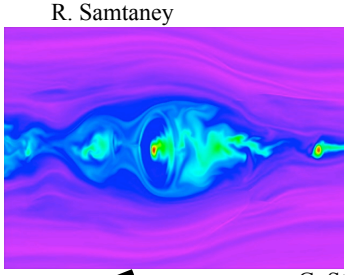


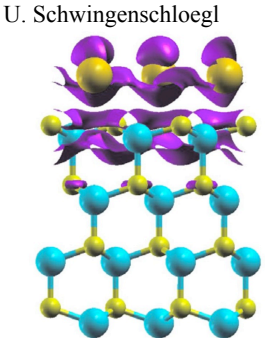


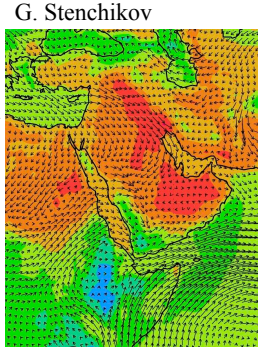


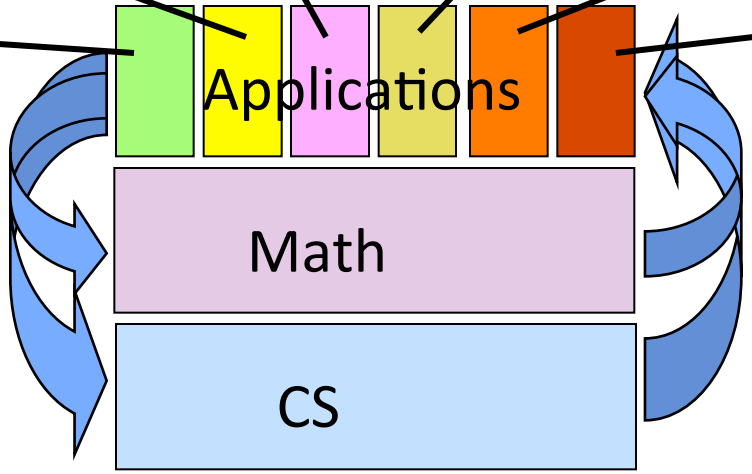












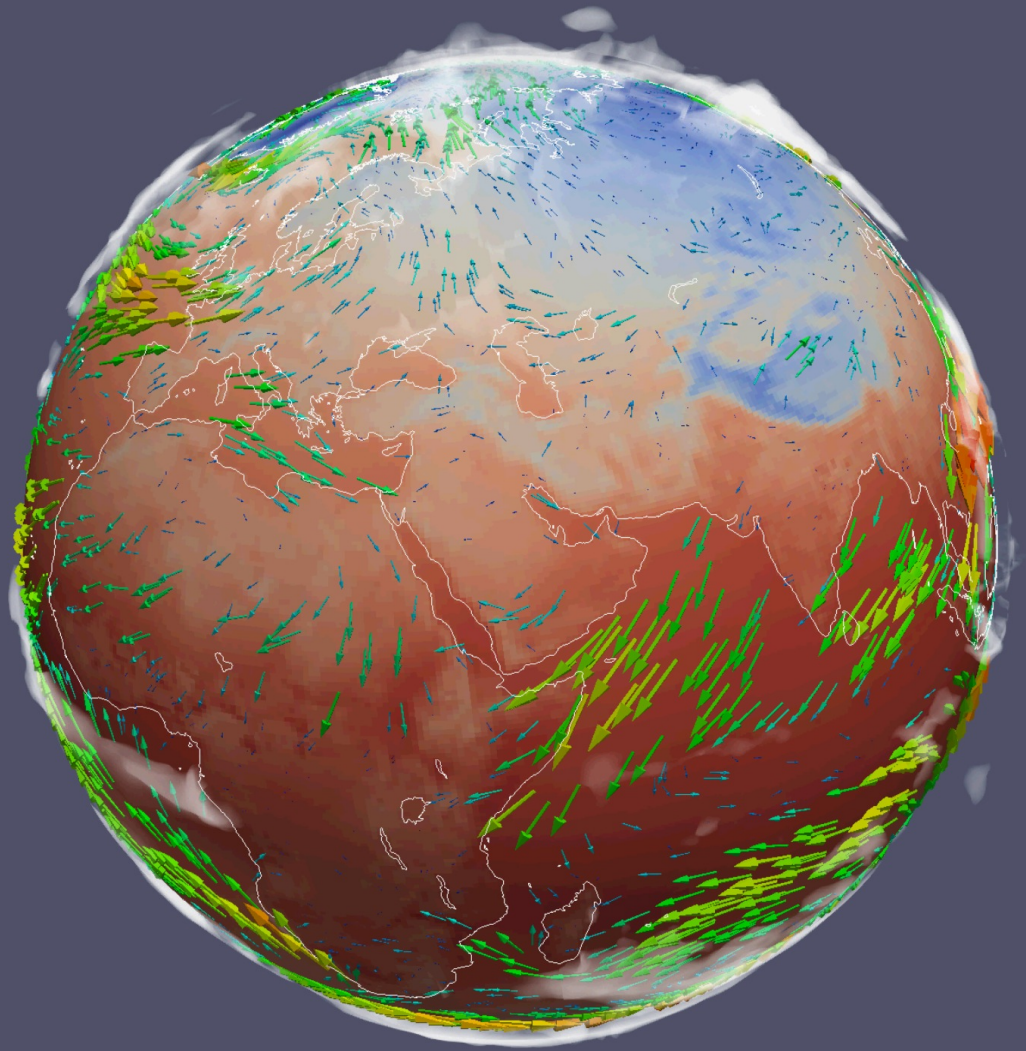
Applications drive

Math & CS enable

Professor Georgiy Stenchikov
Global climate simulation

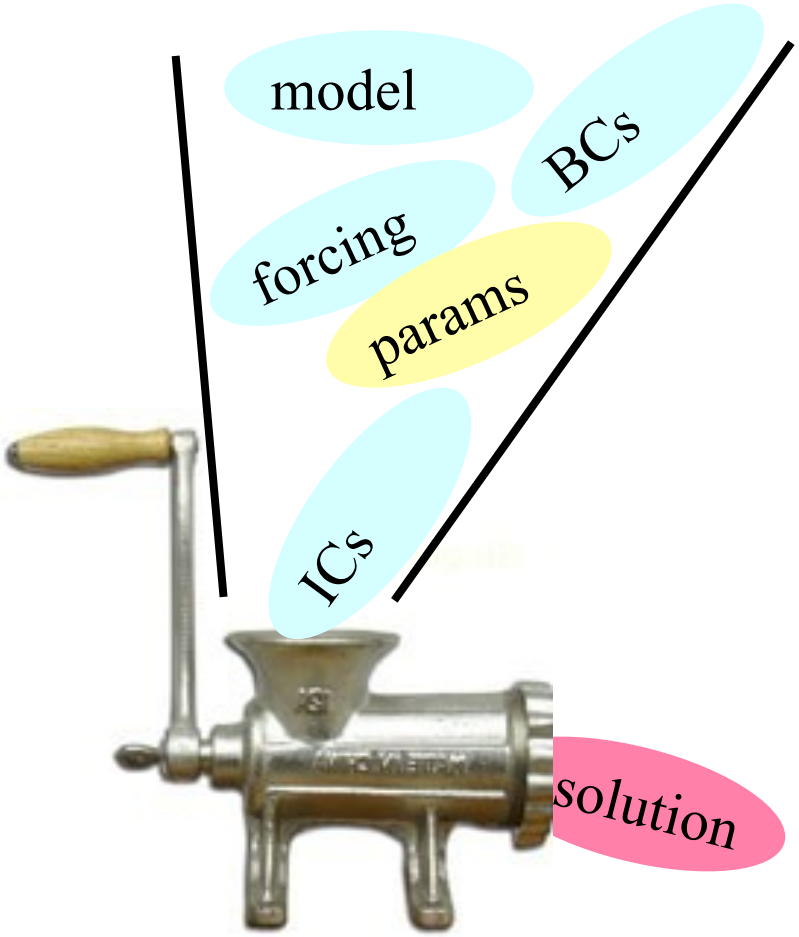
Nobel Prize
(2007, shared)

The KAUST focus within global climate modeling is the transport of aerosols (dust, fine sand, molecules) in the atmosphere. These are *carried* by the climate and, in turn, *affect* the climate.

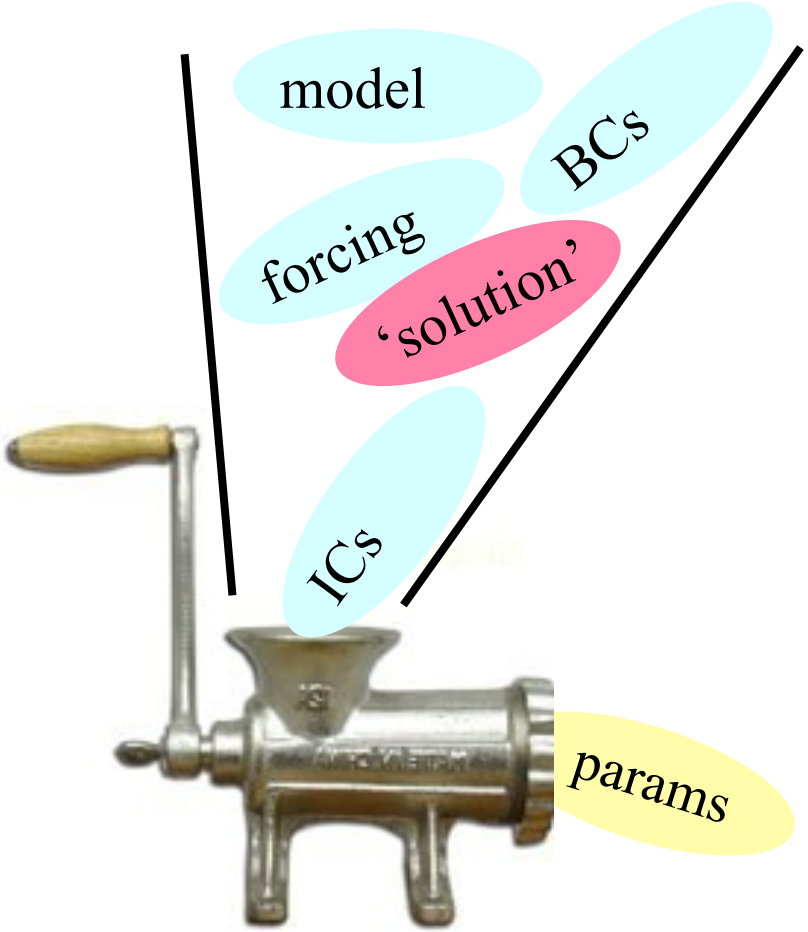


Combining the 3rd and 4th paradigms: forward vs. inverse problems

forward problem



inverse problem



+ regularization

Combining the 3rd and 4th paradigms: data assimilation

Theory

Fully Nonlinear Filters

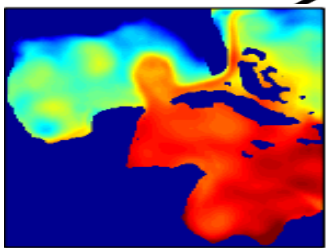
Dual Filters Coupled Models

Robust Ensemble Filters

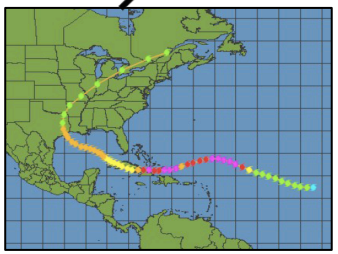
Hybrid Adjoint-Ensemble Filters

Bayesian Filtering **Data Assimilation**

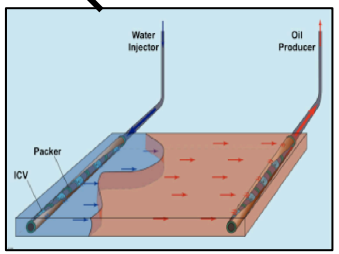
Applications



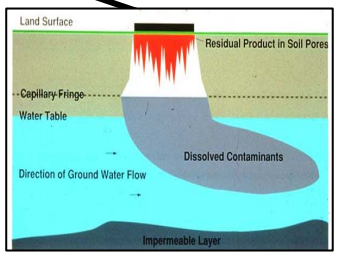
Ocean Circulation



Storm Surge Prediction

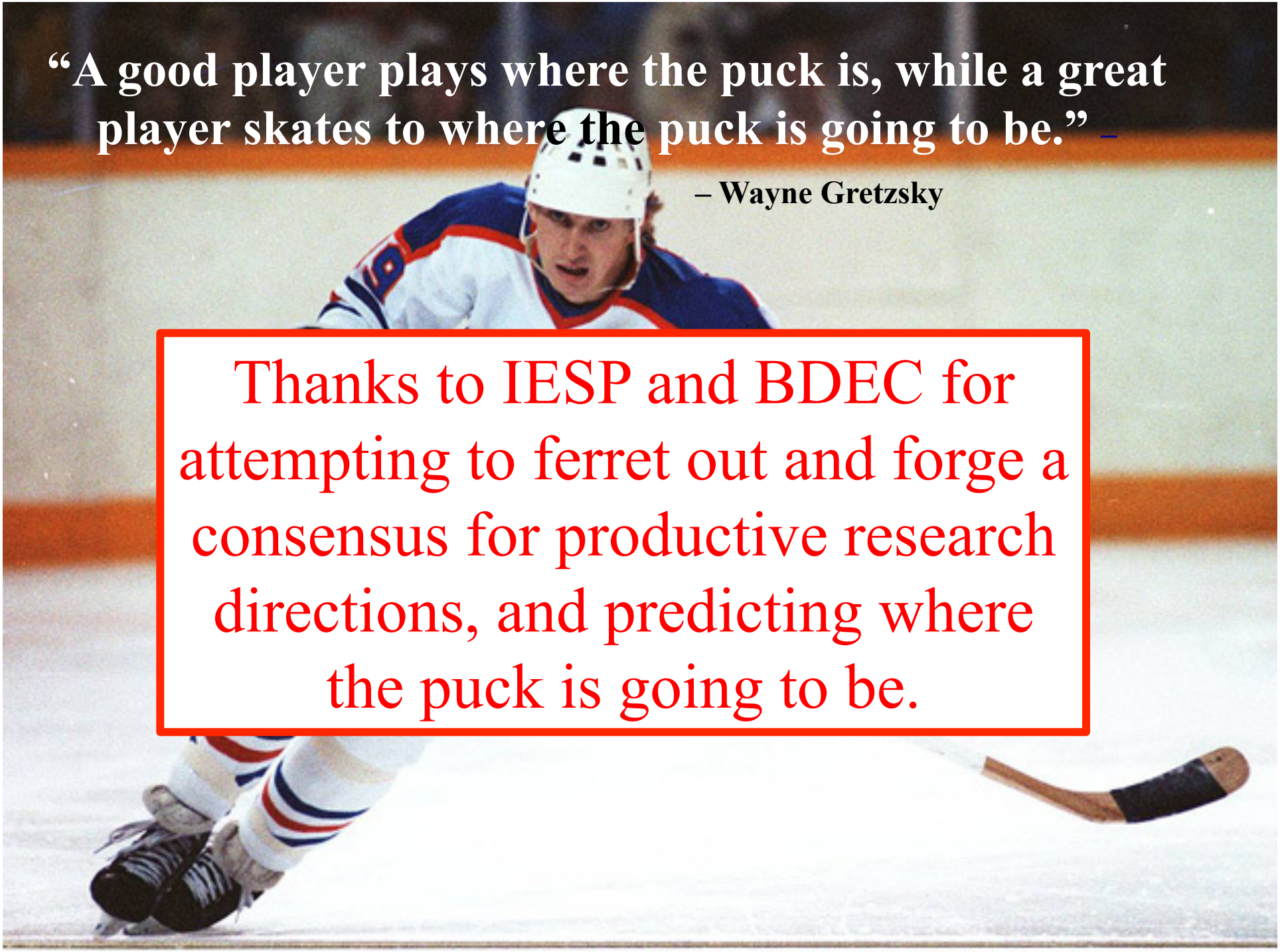


Reservoir Exploitation



Contaminant Transport

c/o I. Hoteit, KAUST


"A good player plays where the puck is, while a great player skates to where the puck is going to be." –
– Wayne Gretzsky
Thanks to IESP and BDEC for attempting to ferret out and forge a consensus for productive research directions, and predicting where the puck is going to be.

جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of
Science and Technology
شكرا
Thank you!