Credit: evv/Shutterstock.com and D-Wave, Inc.

**How NASA-USRA collaborations have advanced knowledge in and with the use of new computing technologies.**

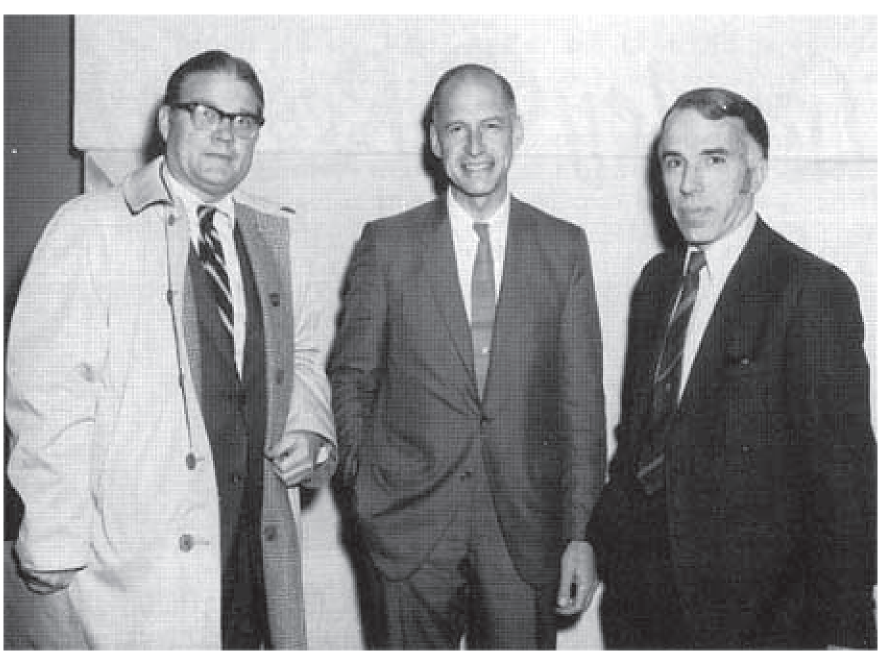
# FROM NUMERICAL ANALYSIS TO QUANTUM COMPUTING

When USRA was created in 1969, its first task was the management of the Lunar Science Institute near NASA's Manned Spacecraft Center (now the Johnson Space Center). A little more than three years later, USRA began to manage the Institute for Computer Applications in Science and Engineering (ICASE) at NASA's Langley Research Center (LaRC). The rationale for creating ICASE was developed by Dr. John E. Duberg (1917-2002), who was the Associate Director at LaRC and later the Chief Scientist at the Center. In February of 1972, Duberg wrote a memorandum to the senior management of LaRC, expressing his view that:

> *The field of computers and their application in the scientific community has had a profound effect on the progress of aerospace research as well as technology in general for the past 15 years. With the advent of "super computers," based on parallel and pipeline techniques, the potentials for research and problem solving in the future seem even more promising and challenging. The only question is how long will it take to identify the potentials, harness the power, and develop the disciplines necessary to employ such tools effectively.*[1]

Twenty years later, Duberg reflected on the creation of ICASE:

> *By the 1970s, Langley's computing capabilities had kept pace with the rapidly developing technology in the hardware. ... [Center staff] recognized that if the Center was to realize to the*



**John E. Duberg, Chief Scientist, LaRC; George M. Low, former head of the Office of Manned Spaceflight at NASA Headquarters; and Edgar M. Cortright, Director of LaRC when ICASE was formed.**

Essay by W. David Cummings. Design by Erin Senoz.

*fullest the world-class computing capability that it had assembled, a more aggressive and basic effort in the science of computing was needed.*[2]

LaRC had already formed one collaborative institute, the Joint Institute for the Advancement of Flight Sciences with George Washington University. Because that experience had been positive, it was decided that a new institute should now be formed, and two weeks after Duberg's internal memo, the Director of LaRC, Edgar Cortright (1923-2014), sent a memo to NASA Headquarters suggesting the establishment of another institute that would:

*Bring together experts in applied mathematics and computer science from universities and industrial establishments for the exploitation of the capabilities at Langley Research Center and to influence through their competence the quality of activity now carried on throughout the Center.*[3]

**James M. Ortega – the founding director of ICASE**

Cortright had been hired by the second NASA Administrator, James Webb, and he had been sent to LaRC by Webb to give the Center "a shot in the arm."[4] As Duberg later reflected, the new institute was to:

*Involve a broad spectrum of universities to maximize the diversity of research interests. It would also increase the number of universities that could avail themselves of superior computing capabilities. Fortunately, it was not necessary to invent any new external mechanism to sponsor this venture. NASA had already encouraged the formation of the Universities Space Research Association (USRA) to manage its program for the analysis of rock samples from the Moon by the broad base of interested researchers that were to be found in the university community.*[5]

**ICASE thrived at LaRC by bringing university researchers on a visiting basis to work in the areas of numerical mathematics, fluid mechanics, and applied computer science**

NASA quickly negotiated a cooperative agreement with USRA for the operation of ICASE, which was formed in July of 1972. The search for a director resulted in the appointment of Dr. James M. Ortega (1932-2008) of the University of Maryland. Ortega had just completed two books on numerical methods: one was titled *Numerical Analysis: A Second Course*; and the other, co-authored with Werner Rheinboldt, was titled *Iterative Solutions of Nonlinear Equations in Several Variables*. Ortega's expertise and his interest in the marriage of computer science and applied mathematics made him an obvious choice to be the founding director of ICASE.

Part of the impetus for the creation of ICASE was the advent of computers that used parallel processing. LaRC was soon to receive delivery of Control Data Corporation's STAR 100 vector processor. The initial program plan for ICASE reflected a merger of LaRC's interest in developing the Center's capabilities using the new supercomputers with Ortega's interests in applied mathematics. Thus, the program plan's four categories:

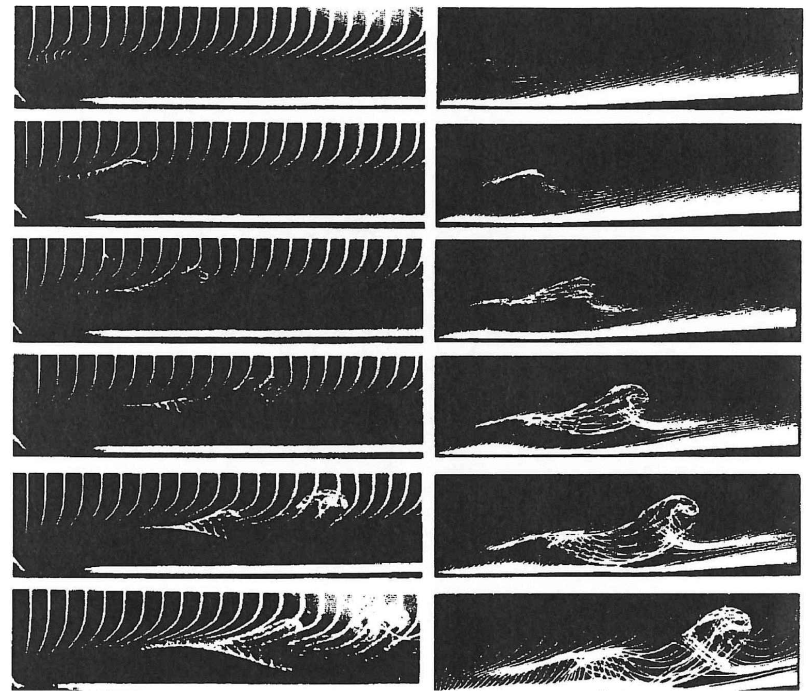

**ICASE staff and visiting scientists during the summer of 1986**

1. Efficient use of vector and parallel computers, with particular emphasis on the CDC STAR-100.
2. Numerical analysis, with particular emphasis on the development and analysis of basic numerical algorithms.
3. Analysis and planning of large-scale software systems.
4. Computational research in engineering and the natural sciences, with particular emphasis on fluid dynamics.[6]

The STAR-100 did not prove to be very successful, but ICASE thrived at LaRC by bringing university researchers on a visiting basis to work in the areas of numerical mathematics, fluid mechanics, and applied computer science. ICASE had a small permanent staff and a cadre of 40 to 50 consultants from universities around the world who would visit the institute for varying periods of time. The staff and visitors could infuse the results of their research into the research programs at LaRC, often by conducting joint research with Langley staff. The challenging, real-world problems at NASA's oldest aeronautical research center were of great interest to academic researchers.

**ICASE has been at the heart of advances in numerical analysis and its applications.**

**-Orszag, 1992**



**Comparison of experiment (left) and ICASE numerical simulation (right) of an evolving boundary layer instability at six successive snapshots.** [8]

Ortega served as Director of ICASE from 1972 to 1977. His successors were Dr. Milton E. Rose (1925-1993), who served from 1977 to 1986; Dr. Robert G. Voigt, who served from 1986 to 1991; Dr. M. Yousuff Hussaini, who served from 1991 to 1996; and Manuel D. Salas, who served from 1996 to 2002.

For the 20th anniversary of ICASE in 1992, Director Yousuff Hussaini identified several of the institute's accomplishments, including:

- Performing the first application of multigrid methods to fluid flow problems
- Developing the first general theory of multigrid methods, using finite elements and the variational formulation
- Pioneering the development of spectral methods in fluid dynamics
- Developing a modern theory of boundary conditions for hyperbolic partial differential equations
- Developing unstructured multigrid strategies for improving efficiency of unstructured flow solvers in both two and three dimensions
- Developing highly effective and computationally tractable techniques for parameter estimation and feedback control
- Developing first nonparallel theories of linear and nonlinear growth of Görtler vortices in incompressible and compressible boundary layer flows [Görtler vortices can occur with flow over curved surfaces, e.g., the wing of an aircraft, and can lead to turbulent flow.]
- Performing the first direct numerical simulation of transition in supersonic boundary layers
- Developing the first compressible subgrid scale

**Milton Rose**

**Robert Voigt**

**Yousuff Hussaini**

**Manuel Salas**

model for compressible turbulence, and performing the first large-eddy simulation of compressible homogeneous turbulence

- Developing new instability modes for high speed reacting mixing layers relevant to scramjets
- Developing the first high-order schemes for acoustics
- Performing seminal work on absorbing boundary conditions, allowing acoustics problems to be treated by standard algorithms
- Conducting pioneering work on parallel algorithms and architectures a decade before commercial parallel machines became available
- Designing and implementing the Finite Element Machine, one of the first Multiple Instruction, Multiple Data architectures and the first to incorporate fast summation hardware[7]

Distinguished members of the applied mathematics research community recognized the success of ICASE in advancing knowledge in numerical methods and in fostering interactions between NASA and the university research community. Dr. Peter Lax of the Courant Institute of New York University wrote:

> *Through its far-flung visitor program, just about every important player in CFD [Computational Fluid Dynamics] spent some time at ICASE; through their interaction the importance of the ideas in this field were clarified.*[8]

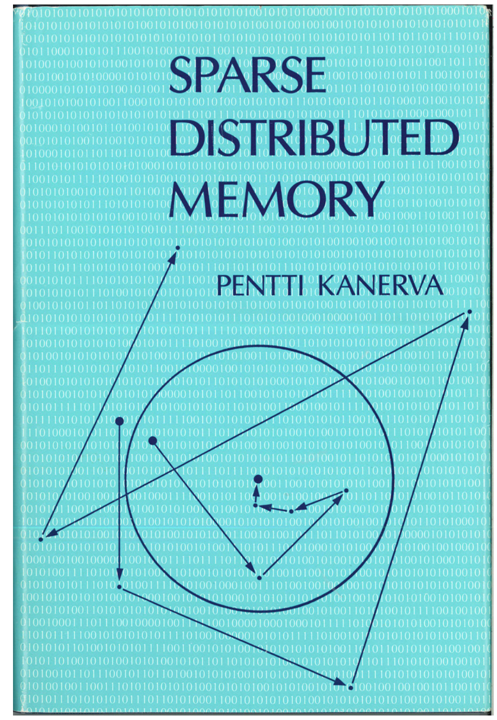
Twenty years after the establishment of ICASE, Professor Steven Orszag (1943-2011) commented:

> *ICASE has been at the heart of advances in numerical analysis and its applications. Many of the great leaps in computational methods have marched to the beat of developments whose genesis was discussed in corridors and focused thinking in the offices of ICASE."*[9]

The success of ICASE led to a request from NASA in 1983 that USRA establish a second computer-oriented institute, this time at NASA's Ames Research Center. NASA Ames was soon to acquire an Intel iPSC Hypercube and Sequent Computing supercomputers. In response to NASA's request, USRA created the Research Institute for Advanced Computer Science (RIACS).


Peter Denning

The founding director of RIACS was Dr. Peter J. Denning, who was a graduate of MIT's Electrical Engineering Department. By the time of his selection as Director of RIACS, Denning had written *Operating Systems Theory* with Edward G. Coffman and *Machines, Languages, and Computation* with Jack B. Dennis and Joseph E. Qualitz. Denning had taught at Princeton and Purdue Universities. He was the Head of the Department of Computer Sciences at Purdue just prior to joining RIACS.



Book authored by RIACS researcher Pentti Kanerva


William Ballhaus

With the support of the Center Director at NASA Ames, Dr. William F. Ballhaus Jr., Denning began to build interdisciplinary teams of computer scientists and NASA scientists and engineers that would tackle some of the hardest problems faced by NASA. The initial research areas at RIACS were computing, networking, and artificial intelligence. In 2014, Denning reflected on the accomplishments of RIACS during his tenure:

> *In the computing area our people helped NASA find new algorithms*

*for efficiently computing fluid flows on parallel machines. An example that caught a lot of attention at the end was a pre-processor for programs targeted for the Connection Machine. The pre-processor mapped grid points on to neighboring CPUs and achieved a speedup over the Cray machines using a Connection Machine that cost 1/10 as much as the Cray.*

*The AI group contributed similarly, and a couple of things stood out for me. One was the research of Dr. Pentti Kanerva and others in the group working on Sparse Distributed Memory (SDM), a memory architecture modeled after the human memory; it was producing results at learned responses better than neural networks at the time. The other was the Bayesian Learning group, which pioneered with the brand-new techniques of Bayesian learning, produced novel results in allied fields especially astronomy, and eventually became the hottest research area in AI.*

*The Networking group got NASA-Ames into the full Internet age and into local networks that could keep up with supercomputers. They also pioneered in telescience, the conduct of scientific operations remotely, which turned into a major networking area in the years following.*

**As an independent institute of a university-based consortium, RIACS accessed a level of research ability in its university members that is unmatched anywhere else.**

**-Hubbard, 2008**

**We were doing what NASA originally chartered us to do, which was to engage in grand challenge areas with them and make progress through computing. We were quite successful.**

**-Denning, 2014**

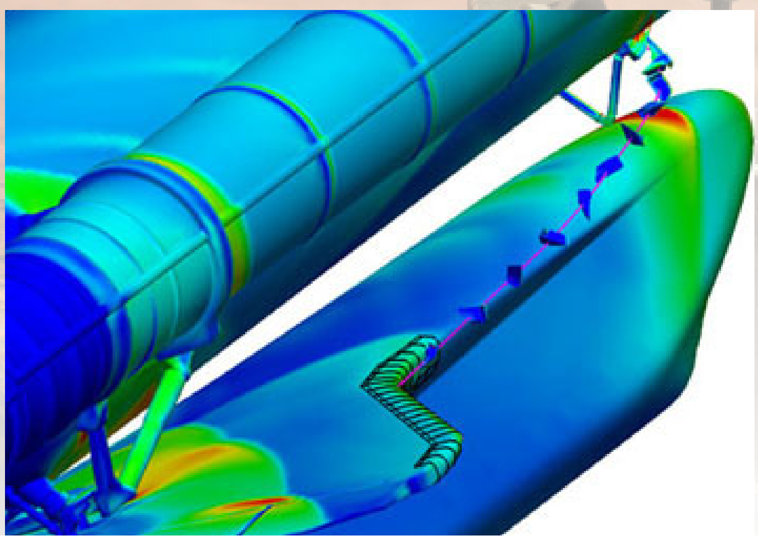
> *We were doing what NASA originally chartered us to do, which was to engage in grand challenge areas with them and make progress through computing. We were quite successful.*[10]

Distinguished members of the NASA and outside research communities agreed with Denning's assessment of RIACS. A former Director of NASA Ames, G. Scott Hubbard, wrote:

> *As an independent institute of a university-based consortium, RIACS accessed a level of research ability in its university members that is unmatched anywhere else. … The tremendous talent of RIACS was regularly tapped by NASA to lead some of our most important efforts. Dr. Walter Brooks, a RIACS staff member, was asked to lead the Columbia Supercomputing effort. He led a team… to acquire the 10,240 processor Columbia Supercomputing System, at the time the fastest computer in the world.*[11]

Douglas R Hofstadter, author of *Gödel, Escher, Bach: An Eternal Golden Braid*, wrote of Kanerva:

> *Sparse distributed memory is among the most inspiring ideas that I have ever encountered in all of cognitive science. … Pentti Kanerva's work on sparse distributed memory points the way to new computing*



Cart3D simulation of the trajectory of tumbling debris from foam and other sources on during the ascent of the Space Shuttle Columbia

> *technologies that can deal with the ubiquitous approximations and blurry categories that characterize the real world and that are intractable to most types of computing technology. More specifically, sparse distributed memory is, in my view, exactly the right kind of software that could underlie the development of highly autonomous robots of the sort that could be sent to explore planets and their moons – a most exciting prospect in many dimensions.*[12]

Nils J. Nilsson, a renowned researcher and author in the field of artificial intelligence, wrote of RIACS scientist Dr. Peter Cheeseman's work on Bayesian Classification:

> *The Bayesian Classification research done by RIACS was quite controversial when it began, but time has definitely proven its soundness and importance through the penetration of Bayesian classification technologies in numerous industries.*[13]

Barry Leiner

Denning served as Director of RIACS from 1983 to 1990. Among his notable successors was Dr. Barry M. Leiner (1945-2003), who served as Director of RIACS from 1999 to 2003. As a manager at the Defense Advanced Research Projects Agency (DARPA) in the early 1980s, Leiner was deeply involved in the evolution of the Internet, particularly in the establishment of a process to determine standards for its organizational structure.

David Bell

After 25 years of innovation at RIACS, its Director, Dr. David Bell, noted a number of successes:

- In 1987 Peter Cheeseman was the principal developer of AutoClass, which was the first AI software to make a published astronomical discovery. Given real valued or discrete data, AutoClass determines the most probable number of classes present in the data, the most probable descriptions of those classes, and each object's probability of membership in each class.[14]
- Remote Agent was the first AI software to control a spacecraft in deep space and was the 1999 NASA Software of the Year co-winner.
- In 2002, Cart3D was named the NASA Software of the Year co-winner. RIACS visiting scientist Professor Marsha Berger of the Courant Institute, New York University, was co-inventor of Cart3D, which played a critical role in resolving the main physical cause of the Space Shuttle Columbia disaster–foam debris that struck the orbiter on ascent–by generating simulations that predicted the trajectory of tumbling debris from foam and other sources.[15]

- In collaboration with NASA scientists and engineers, RIACS scientists led the development of MAPGEN, a ground-based mixed-initiative, human-in-the loop control system used to generate activity plans for the Mars rovers. In 2004, MAPGEN became the first artificial intelligence software to plan the work of robots on another planet. RIACS scientist, Dr. Ari Jónsson, was the lead inventor of EUROPA, a constraint-based planning and scheduling engine that lies at the heart of the MAPGEN application.[16]

The work of RIACS scientists Peter Cheeseman on AutoClass and Ari Jónsson on Remote Agent and EUROPA/MAPGEN are examples of optimization problems that are of great interest to NASA. The space agency often needs to find solutions to similar optimization problems, not only for planning and scheduling, but also for software verification and validation, spacecraft power allocation, image analysis, machine learning and many other artificial intelligence problems.

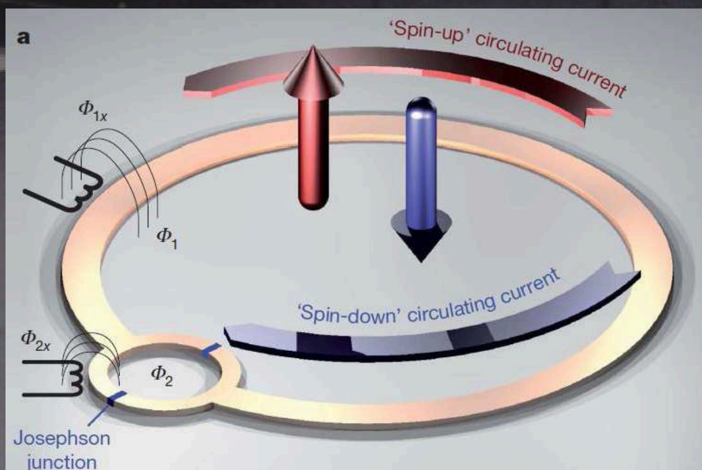
In 2012, USRA entered into a joint Space Act Agreement with Google and NASA to conduct collaborative research on the benefits of quantum computing for a range of applications, but particularly for optimization problems. For the collaboration, USRA obtained from D-Wave Systems, Inc., a D-Wave quantum computer, which was installed in the NASA Advanced Supercomputing facility at NASA Ames. USRA manages the science operations for the collaboration, which includes an allocation of 20% of the computing time for the research community through a competitive selection process.

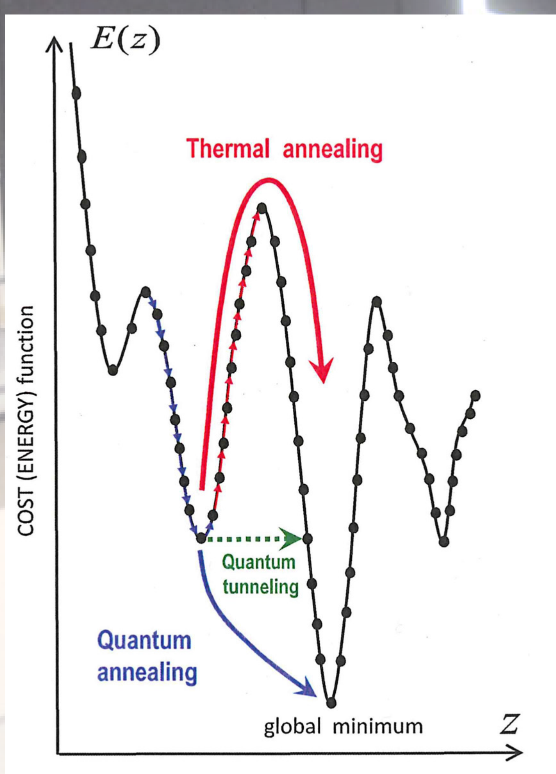
One way that the D-Wave quantum computer can be used to solve optimization problems is as a superconducting quantum annealing machine. In the ordinary annealing of a piece of metal, one heats the metal until it glows and then allows it to slowly cool. The heating frees the metal of discontinuities in its lattice structure, and the cooling allows the atoms in the metal to reform in a more perfect lattice structure that corresponds to the lowest energy state of the metal.

In superconducting quantum annealing, getting the solution to an optimization problem corresponds to finding the lowest energy state of an array of interacting quantum mechanical spin vectors. In the D-Wave computer, the spins are produced by loops of niobium metal maintained near absolute zero temperature so that they can carry quantized superconducting currents. The quantized currents produce quantum bits, called qubits. The current loops are arranged in arrays that are coupled so that the qubits can exchange information. Small external currents produce magnetic fluxes that allow the array of coupled cubits to be programmed, so that a particular optimization problem can be encoded.

The metallic loops contain Josephson junctions, which have insulating separations that force the electronic current to “tunnel” from one side of the junction to the other. The presence of this quantum effect enables the system of interacting spins to be prepared initially into a superposition of states that facilitates exploration of the energy landscape. In regular annealing, this corresponds to the initial heating of the metal. Several controllable, local magnetic fields are then gradually changed to decrease tunneling probabilities (corresponding to cooling of a metal sample during annealing), and the system of interacting spins is “frozen” into its minimum energy configuration, which gives the solution to the optimization problem with high probability.

Credit: NASA/D-Wave, Inc.




Davide Venturelli
USRA Quantum Scientist
Expert in quantum coherence analysis

Kostya Kechedzhi
USRA Quantum Scientist
Expert in superconducting qubit noise

Zhihui Wang
Visiting Scientist, University of Southern California
Expert in D-Wave simulation/benchmarking

**Top image: A simplified schematic of a superconducting flux qubit acting as a quantum mechanical spin. Circulating current in the qubit loop gives rise to a flux inside, encoding two distinct spin states that can exist in a superposition.[18]**

**Bottom image: Energy landscape for a binary optimization problem. Black points correspond to different configurations of binary variables. In quantum annealing, the landscape can be explored through quantum tunneling, as well as thermally.[19]**

**Background image: The D-Wave 2X™ Quantum Computer in the NASA Advanced Supercomputing Facility at NASA's Ames Research Center.**

USRA collaborates with Google and NASA in the operation of the Quantum Artificial Intelligence Laboratory at NASA Ames. As is always the case with research programs, progress is made through the excellence of individual researchers. In this instance, RIACS researchers Dr's Davide Venturelli, Kostya Kechedzhi and Zhihui Wang have helped to provide the needed expertise for USRA's part of the collaboration.

The initial efforts of the USRA team have been to characterize the performance of the D-Wave computer, e.g., to explore the effect of noise on quantum annealing, to demonstrate quantum enhancement over classical methods, and to examine small but very difficult optimization problems.

The first eight proposals that were accepted by USRA for use on the D-Wave quantum computer were from principal investigators at Mississippi State University, the University of Southern California, and the University of California, San Diego, and from universities in Canada, Italy, Mexico, and Switzerland. Research topics from the university research community ranged from condensed matter and quantum annealing device physics to machine learning and network optimization.

The experience of one of the researchers, Dr. Immanuel Trummer of the Swiss Federal Institute of Technology Losanne, illustrates the value of USRA's role in the Quantum Artificial Intelligence Laboratory to individuals and, ultimately, to US leadership in high-technology endeavors. In the spring of 2016, Trummer wrote the note on the right to Drs. Bell and Venturelli.

At this writing, Dr. Trummer is an Assistant Professor at Cornell University, and he is continuing his collaboration with quantum computer scientists at RIACS.

**From: Immanuel Trummer**
**Sent: Thursday, April 07, 2016 6:17 PM**
**To: Bell, David; Davide Venturelli**
**Subject: Update: Paper & Job Search - Thanks!**

**Dear David, dear Davide,**
**I hope you are doing well**
**Good news: our paper on quantum annealing has finally been accepted at VLDB2015, one of the two main database conferences. Thanks so much for all the comments and hints! I'm currently interviewing for tenure track professor positions in computer science in the US and Europe. It's going very well (first offers from Cornell and Maryland and I expect more in the next weeks) and one of the research projects in my portfolio that is attracting significant attention is the work on D-Wave.**

**Thanks so much for giving me the opportunity to make that happen!**
**...**
**Thanks a lot and best wishes,**
**Immanuel**

Far-sighted NASA leaders such as James Webb, Edgar Cortright, and William Ballhaus recognized the value of collaborating with USRA on challenging problems. Their foresight has paid off time and time again, and there are hardly better examples than the advances made in the computational sciences from numerical analysis at ICASE to quantum computing at RIACS.

[1] Hussaini, M. Y. (1993). *ICASE twenty-year anniversary publication*. Columbia, MD: Universities Space Research Association, p. i.

[2] Duberg, J. E. (1993). Some remarks on the founding of ICASE. In *ICASE twenty-year anniversary publication*, pp. 2-6. Columbia, MD: Universities Space Research Association, pp. 4-5.

[3] Hussaini, M. Y. (1993). *ICASE twenty-year anniversary publication*. Columbia, MD: Universities Space Research Association, p. i.

[4] Hansen, J. R. (1994). *Spaceflight Revolution: NASA Langley Research Center from Sputnik to Apollo*. U.S. Government Printing Office: NASA SP-4308, p. 397.

[5] Op. cit. Duberg, 1993. p. 5.

[6] Op. cit. Hussaini, 1993, p. ii.

[7] Ibid., pp. 8-14.

[8] Hussaini, M. Y. (1995). ICASE: NASA Langley's CSE center. *Computational Science and Engineering, IEEE*, *2*(1), p. 8.

[9] Ibid., p. 12.

[10] Denning, P. J. (2014) Personal communication, 24 December 2014.

[11] G. Scott Hubbard to Jennifer Lo, 27 May 2008. Letter in support of the nomination of RIACS for the National Medal of Technology and Innovation. USRA Archives.

[12] Douglas R. Hofstadter to Jennifer Lo, 23 May 2008. Letter in support of the nomination of RIACS for the National Medal of Technology and Innovation. USRA Archives.

[13] Nils J. Nilsson to Jennifer Lo, 22 May 2008. Letter in support of the nomination of RIACS for the National Medal of Technology and Innovation. USRA Archives.

[14] Cheeseman, P., Self, M., Kelly, J., Stutz, J., Taylor, W., and Freeman, D. (1988). AutoClass: A Bayesian classification system. In *Proc. Fifth Int'l Conf. Machine Learning*, pp. 607-611. Palo Alto, CA: Association for the Advancement of Artificial Intelligence.

[15] Bell, D. (2008). *RIACS: 25 Years of Innovation*. Columbia, MD: Universities Space Research Association.

[16] Ibid., pp. 10 and 13.

[17] Bell, D. (2016). Personal communication. Note from Dr. Immanuel Trummer.

[18] Johnson, M. W., Amin, M. H. S., Gildert, S., Lanting, T., Hamze, F., Dickson, N., Harris, R., Berkley, A. J., Johansson, J., Bunyk, P., Chapple, E. M., Enderud, C., Hiltin, J. P., Karimi, K., Ladizinsky, E., Ladizinsky, N., Oh, T., Perminov, I., Rich, C., Thom, M. C., Tolkacheva, E., Truncik, C. J. S., Uchailin, S., Wang, J., Wilson, B., and Rose, G. (2011). Quantum annealing with manufactured spins. *Nature*, *473*, pp. 194-198. Figure 1a.

[19] Smelyanskiy, V. N., Rieffel, E. G., Knysh, S. I., Williams, C. P., Johnson, M. W., Thom, M. C., Macready, W. G., and Pudenz, K. L. (2012). A near-term quantum computing approach for hard computational problems in space exploration. *arXiv preprint arXiv:1204.2821*. Figure 2a.