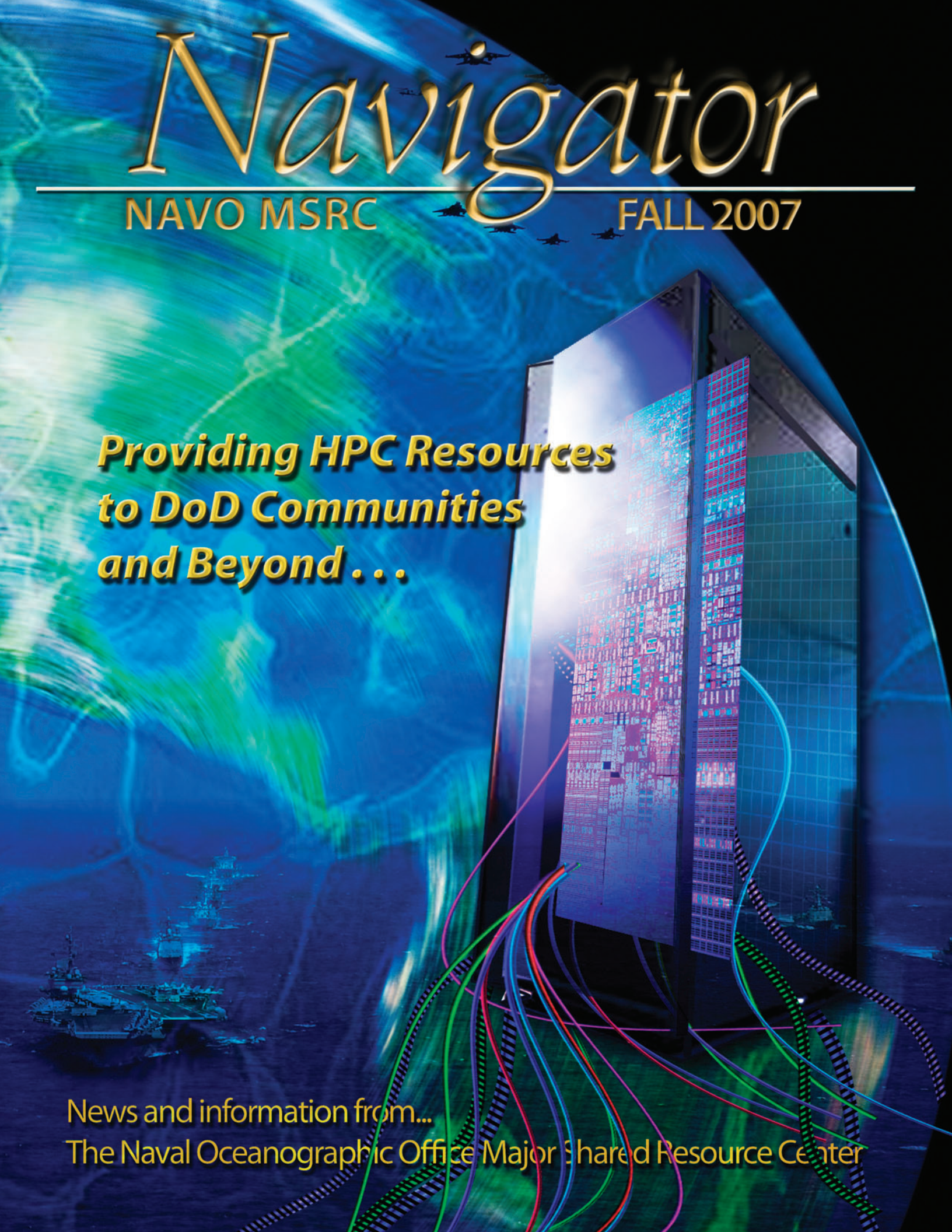
Navigator

NAVO MSRC FALL 2007



Providing HPC Resources to DoD Communities and Beyond . . .

News and information from...
The Naval Oceanographic Office Major Shared Resource Center

The Team Behind the Curtain

Christine Cuicchi
Computational Science and Applications Lead,
NAVO MSRC

A wall of blue curtains extends along the entrance to our machine room, camouflaging the presence of a portion of the support infrastructure for the High Performance Computing (HPC) systems located there. We'd like to pull back the blue curtain of the NAVO MSRC and reveal the team that works to keep our center one of the top supercomputing centers in the world.

As some user services are consolidated across the High Performance Computing Modernization Program (HPCMP), our center is redefining its role in supporting the Program and its user community. The center is always growing, changing, and working diligently to meet the needs of the users, the program, and the Department of Defense. We continue to provide Tier 2 and Tier 3 support to our users. Our center staff strives to attain the height of technical knowledge and expertise across numerous disciplines in order to develop and maintain a dependable, leading-edge high performance computing infrastructure for our users.

In response to user requests and suggestions, we have revamped our website to provide users a more thoughtfully organized interface to the center. And in response to the HPCMP's recognition of a need for real-time computing, a team of developers has been working to create a secure, web-based system for requesting dedicated time on a portion of our P4+ system, KRAKEN. This reservation request system will be deployed in the fall of 2007.

The NAVO MSRC is co-lead on the new HPCMP-wide Mass Storage Initiative, and we are using our current experience in providing a combined 7.8 petabytes in both archival and hardened remote storage to craft an innovative and forward-thinking solution for this ever-growing problem.

The center also provides HPC support and resources to the Navy's Meteorology and Oceanography (METOC) community. This METOC community relies on the NAVO MSRC's well-established HPC system stability and uptime to develop climate, weather, and ocean forecast products that are pushed to a variety of customers around the clock.

In addition to a number of talented HPC, storage, and queuing system administrators, we also have a contingent of operator staff in place 24 hours a day, 7 days a week to provide constant monitoring of center systems and to ensure that after-hours problems are handled swiftly.

A small but dedicated NAVO MSRC team has worked for several months to organize and produce the largest exhibit presence the HPCMP has ever had on the Supercomputing Conference (SC07) show floor—bringing together Major Shared Resource Centers, Allocated Distributed Centers, and HPCMP initiatives together in an information-rich environment in a 40 x 50 foot floor space in the Research Exhibit area.

In short, our team is dedicated to meeting and exceeding the needs of the HPCMP. We hope you've enjoyed the glance behind the curtain, and we look forward to continuing to provide excellent HPC services and support to the DoD HPCMP.

The Naval Oceanographic Office (NAVO) Major Shared Resource Center (MSRC): Delivering Science to the Warfighter

The NAVO MSRC provides Department of Defense (DoD) scientists and engineers with high performance computing (HPC) resources, including leading edge computational systems, large-scale data storage and archiving, scientific visualization resources and training, and expertise in specific computational technology areas (CTAs). These CTAs include Computational Fluid Dynamics (CFD), Climate/Weather/Ocean Modeling and Simulation (CWO), Environmental Quality Modeling and Simulation (EQM), Computational Electromagnetic and Acoustics (CEA), and Signal/Image Processing (SIP).

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NAVO MAJOR SHARED RESOURCE CENTER

- Providing over 58 teraflops of computing power to the DoD HPCMP user community
  - IBM P5+ - Babbage - 22 Tflops/3072 processors
  - IBM P5+ - Pascal - 14 Tflops /1920 processors
  - IBM P4+ - Kraken - 19 Tflops/2944 processors
  - IBM P4+ - Romulus - 3 Tflops/512 processors

HPC - It's about Data & Information!

- Providing 3.6 Petabytes of storage to the user community

- Providing over 4.15 Petabytes of hardened remote storage.

-Providing specialized 24x7 support to the Naval Meteorology and Oceanography (METOC) operational forecasting community

Solving the hard problems...

DoD HPC Modernization Program

Design of Energetic Ionic Liquids

Jerry A. Boatz, Air Force Research Laboratory, Space and Missile Propulsion Division, Edwards AFB, CA
Hui Li, Department of Chemistry, University of Nebraska-Lincoln
Mark S. Gordon, Department of Chemistry, Iowa State University

An essential need of the U.S. Air Force is the discovery, development, and fielding of new, energetic materials for advanced chemical propulsion in rocket and missile applications. Some of the key factors driving the requirement for new chemical propellants include (a) improved performance in terms of increased specific impulse and density, (b) reduced sensitivity to external stimuli such as impact, friction, shock, and electrostatic discharge, and (c) mitigation of environmental and toxicological hazards (and the resulting costs) associated with currently used propellants.

A class of compounds that can potentially meet these requirements is known as ionic Liquids (ILs), which are chemical salts with unusually low melting points. The physical and chemical properties of ILs render them useful for many purposes, most notably as environmentally benign ("green") solvents/reaction media but also as catalysts, electrolytes, etc.[1] From a Department of Defense (DoD) perspective, ILs are being explored as new propellants, explosives, and munitions.[2]

The Air Force, in particular, is interested in ILs as potential replacements for currently used monopropellants such as hydrazine, which is carcinogenic, highly toxic, and has relatively modest performance characteristics.

In contrast, many ILs have superior densities and specific impulses as well as significantly reduced sensitivity and toxicity characteristics. Furthermore, their properties can be carefully tuned via the choice of the component ions.

The overall objective of the Design of Energetic Ionic Liquids challenge project is to address several key technical issues and challenges associated with the characterization, design, and development of ILs as new monopropellants. Among these, for example, are a fundamental understanding of the (in)stability of ILs, the intrinsic nature of the short- and long-range structure and interactions between the component ions, [2e-f] and identification of the key steps in the initial stages of decomposition and combustion. [2a-c] The research described in this article is focused on characterization of the structures and stabilities of ion pair clusters and prediction of their interaction energies in the gas phase.

Our computational approach utilizes quantum chemical methods for prediction of ion pair structures and

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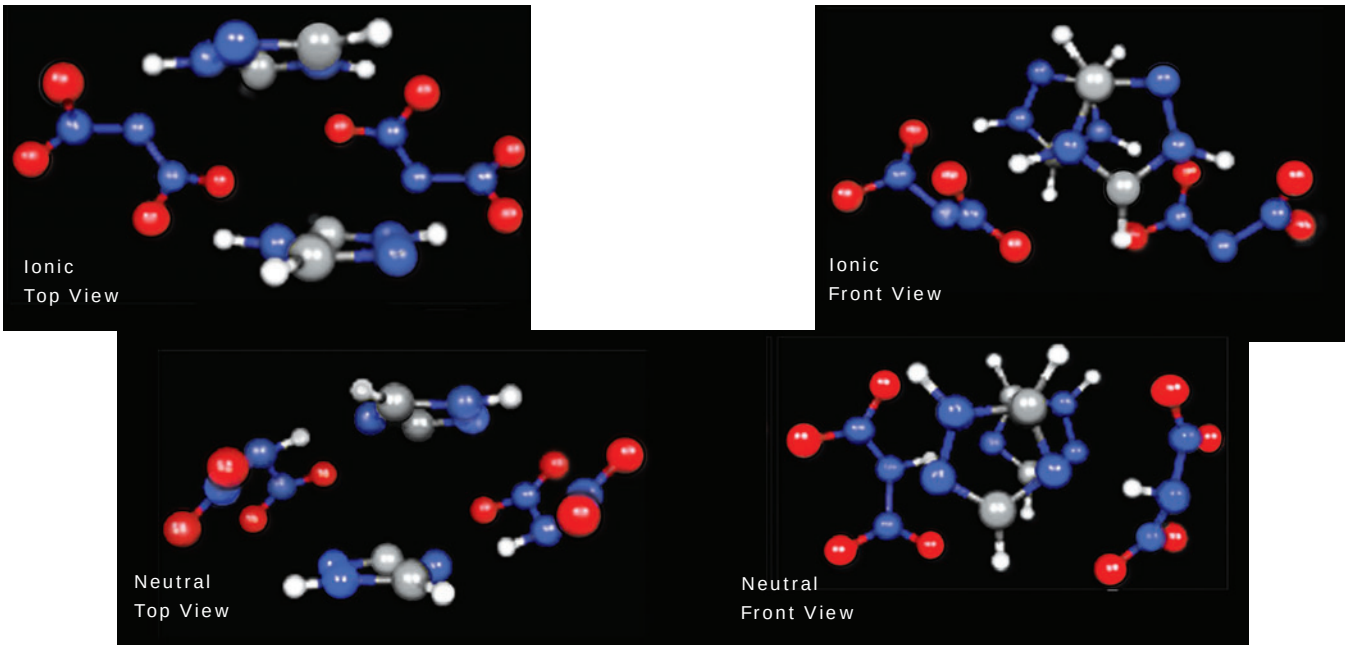

Figure 1. MP2/aug-cc-pVDZ optimized structures of two pairs of 1,2,4-triazolium (1,2,4-triazole) and dinitramide (dinitramine) molecules. H is white, C is gray, O is red, N is blue.

interaction energies. In particular, geometry optimizations were performed using second-order perturbation theory[3] (MP2, also known as MBPT2) with the aug-cc-pvdz basis set,[4] denoted as MP2/aug-cc-pvdz.

Relative energies were refined using a systematic series of single-point energy calculations at the MP2 and coupled cluster (e.g., singles and doubles with a perturbative estimate of triples, CCSD(T)[5]) levels of theory. Specifically, MP2/cc-pvdz, MP2/aug-cc-pvdz, and CCSD(T)/cc-pvdz energy calculations were combined to obtain estimated CCSD(T)/aug-cc-pvdz relative energies. All computations were performed using the GAMESS quantum chemistry code.[6]

MP2 and coupled cluster (CC) calculations in GAMESS utilize a library of communications routines known as the Distributed Data Interface (DDI),[7] a high-level communications layer operating between GAMESS and the underlying message-passing protocols (Shared Memory (SHMEM), Message Passing Interface (MPI), Low-level Application Programming Interface (LAPI), or sockets within a Transmission Control Protocol/Internet Protocol (TCP/IP) stack.)

In the case of the Naval Oceanographic Office Major Shared Resource Center (NAVO MSRC) IBM systems KRAKEN and BABBAGE, DDI uses MPI for intranode communications and the LAPI protocol for messages between nodes. These types of calculations have significant memory requirements and therefore are well suited for execution on systems with large amounts of memory per node, such as BABBAGE.

Coupled cluster calculations are especially memory intensive and, as implemented in GAMESS with DDI, utilize a threefold hierarchy of memory. First, a modest amount of Replicated Data (RD) is exclusively assigned to each core. Similarly, a block of Node-specific Data (ND) is reserved on each node and is shared by all the cores on that node. The remaining memory on each node is collectively shared by all cores as a large, single pool of Distributed Data (DD). Therefore, the required Memory (M_{CC}) per node for CC calculations is $M_{CC} = P*(RD) + (ND) + (DD)/N$, where "P" and "N" are the number of cores per node and the total number of nodes, respectively, used in the computation.

Basis Set (# of AOs)	RD (MW/core)	ND (MW/node)	DD (MW)	P	N	MCC (MW/node)
cc-pvdz (376)	8	1,175	4,950	16	64	1,381
6-311++G(d,p) (580)	22	3,298	16,000	16 1 16	64 64 2	3,900b 3,570b 11,474c
aug-cc-pvtz (1268)	26	3,875	19,150	1 1	64 2	4,200b 13,476c
aug-cc-pvqz	330	18,493	146,000	1 1	64 2	21,105b 91,823d
aug-cc-pvqz (2228)	2495	60,370	807,000	1 1	64 2	75,475b 466,365d

a. "MW" denotes megawords. (106 64-bit words)
b. Exceeds amount of usable physical memory on each standard node. (See Table 2)
c. Fits within usable physical memory on each bigmem node, but execution time is prohibitively long.
d. Exceeds amount of usable physical memory on each bigmem node. (See Table 2)

Table 1. Memory requirements for CCSD(T) single point energy calculations.

The values of RD, ND, and DD are determined by the specifics of the calculation, whereas suitable values of P and N are dictated by the hardware, specifically, the amount of accessible physical memory per node. If necessary, P can be chosen to be smaller than the number of available cores per node Pmax in order to reduce the amount of required memory per node. Table 1 summarizes the memory requirements for CCSD(T) calculations using a series of increasingly large basis sets.

Only the smallest calculation (CCSD(T)/cc-pvdz) could be performed within the constraints of the hardware (P_{max} and M_{max}) and the challenge queue limits (N_{max} and T_{max}, see Table 2.) In principle, the CCSD(T)/6-311++G(d,p)[8] and CCSD(T)/aug-cc-pvdz calculations could be run on the pair of "bigmem" nodes, but the estimated required wall time of the former, on the order of 100 days, is prohibitively long. Conversely, this calculation would be within the realm of practicality if ~100 bigmem nodes were available.

One of the specific ion combinations considered in this work is the 1,2,4-triazolium cation ($[C_2N_3H_4]+$) paired with the dinitramide anion ($[N(NO_2)_2]-$). Of the numerous structures found for the two pairs of 1,2,4-triazolium and dinitramide ions, or the pairs of corresponding neutral 1,2,4-triazole and dinitramine molecules, the most stable MP2/aug-cc-pvdz optimized geometries are shown in Figure 1.

In the ionic structure, each 1,2,4-triazolium forms two hydrogen bonds, via the hydrogens on the N atoms, to the O atoms of the dinitramide ions. Interestingly, this structure exhibits parallel stacking of the two cationic 1,2,4-triazolium rings. The interplane distance is ~3.2 Å, with a parallel displacement of ~1.4 Å. The corresponding neutral tetramer shows a similar parallel stacking arrangement of the triazole rings.

Furthermore, it is of interest to determine the cluster size at which the ion pair structures become more stable than the corresponding neutral pair structures. A previous study predicted that ion pair dimers are typically higher in energy than neutral pair dimers.[2c] Including zero point vibrational energy (ZPVE) corrections, the ionic tetramer in Figure 1 is 1.2 kilocalorie/mole (kcal/mol) lower than that of the neutral one.

The MP2 method tends to predict higher energies for ionic species vs. neutral species,[2c] so more accurate CCSD(T)/aug-cc-pVDZ energy calculations of these two tetramer structures were desired. However, since the computational cost of CCSD(T)/aug-cc-pVDZ is prohibitive, these energies were approximated from the MP2/aug-cc-pVDZ energies by estimating the electron correlation energy differences using three independent methods: (1) the differences between the MP2/cc-pVDZ and CCSD(T)/cc-pVDZ energies of the tetramers, (2) the differences between the MP2/aug-cc-pVDZ and CCSD(T)/aug-cc-pVDZ energies of the twelve pairs of dimers in these two tetramers, and (3) the differences between the MP2/aug-cc-pVDZ and CCSD(T)/aug-cc-pVDZ energies of the eight monomers in these two tetramers. Using these three methods, and including ZPVE corrections, the estimated CCSD(T)/aug-cc-pVDZ energy of the ionic tetramer is lower than that of the neutral tetramer by 5.7, 7.3, and 7.7 kcal/mol, respectively.

In conclusion, quantum chemical calculations suggest that cation-cation parallel stacking structures can exist in very small ionic clusters such as two 1,2,4-triazolium cations and two dinitramide anions. Furthermore, for two pairs of 1,2,4-triazolium and dinitramide, ionic structures are more stable than the corresponding neutral structures.

Finally, it should be noted that lower theoretical methods, do not include the effects of electron correlation, such as Hartree-Fock, do not predict a parallel stacking geometry of the rings. Therefore, it is essential to utilize correlated methods such as MP2 and CCSD(T) in order to obtain proper descriptions of the structures and interaction energies of these ion clusters. The structural motifs and interaction patterns found in this study provide new understanding of ionic materials with aromatic rings.

Queue	Cores per node (Nmax)	Maximum # of nodes (Nmax)	Maximum memory/node Mmax (MW/node)	Maximum wall time Tmax (hours)
Challenge	16	64	~3,500	48
Bigmem	16	2	~15,500	48*

a. "MW" denotes megawords. (106 64-bit words)
* 48 hour limit obtained via special request. The default wall time limit of the bigmem queue is 12 hours.

Table 2. Challenge and bigmem queue characteristics on BABBAGE.

Acknowledgments

A grant of computer time from the Department of Defense High Performance Computing Modernization Program Office at the Naval Oceanographic Office Major Shared Resource Center (NAVO MSRC), in conjunction with the Design of Energetic Ionic Liquids challenge project, is gratefully acknowledged. This work was supported by the Air Force Office of Scientific Research (AFOSR) and the Air Force Research Laboratory, Space and Missile Propulsion Division. The technical assistance of Mr. John Skinner, NAVO MSRC, is deeply appreciated.

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Supporting the Navy's METOC Operational Community

Christine Cuicchi, Computational Science and Applications Lead, NAVO MSRC
Dr. Frank Bub, Ocean Modeling Technical Lead, Naval Oceanographic Office

The NAVO MSRC serves a unique function within the HPCMP: the center supports the Navy's Meteorology and Oceanography (METOC) operational forecasting community on a 24 hours a day, seven days a week basis.

The METOC operational forecasting group located at the Naval Oceanographic Office (NAVOCEANO) run a number of oceanographic models on the unclassified and classified HPC systems at the center in order to provide oceanographic forecast products to the Navy's fleet.

NAVOCEANO operational modelers run a number of models from the Computational Technology Areas (CTA) of Climate Weather Ocean (CWO) and Computational Fluid Dynamics (CFD) on NAVO MSRC HPC systems several times a day. These applications include the Modular Ocean Data Assimilation System (MODAS), Relocatable Navy Coastal Ocean Model (RELO NCOM), the Navy Coupled Ocean Data Assimilation System (NCODA), the Global Navy Coastal Ocean Model (NCOM), the Shallow Water Assimilation Forecast System (SWAFS), the Wave Analysis Model (WAM), and the Simulating Waves Nearshore model (SWAN).

High performance computing resources are required as these models are run not only numerous areas of interest throughout the world's oceans, but also at varying resolutions, some of which are as high as 1/50th degree resolution.

These model products assist fleet ships in numerous ways, including providing information that helps in adjusting side scan sonar and other survey equipment for specific local hydrographic conditions.

These products also help the ships to plan and adjust travel routes in anticipation of adverse weather and sea conditions. The Navy's fleet is not alone in relying on the products produced on NAVO MSRC computers—the operational forecast products and analyses are pushed to numerous entities within the Department of Defense.

While this operational forecast support is provided year-round, there have been instances where the METOC community has relied particularly heavily on the NAVO MSRC's resiliency and reliability. In 2006 and 2007 the NAVO MSRC rearranged its preventative maintenance schedule

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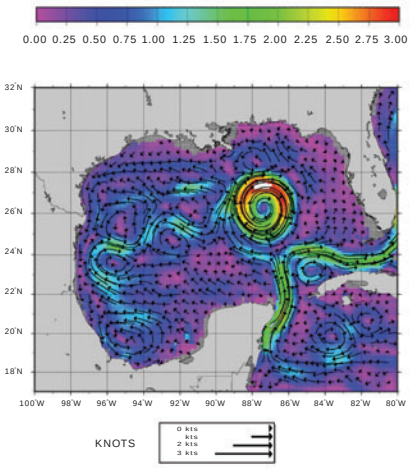
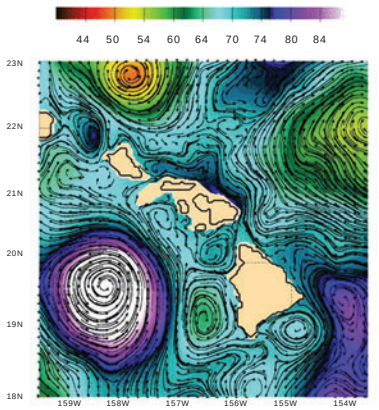


Navy Coastal Ocean Model glb Domain
Currents at 00100 meters 036 hr FORECAST valid 10 OCT 07 1200Z



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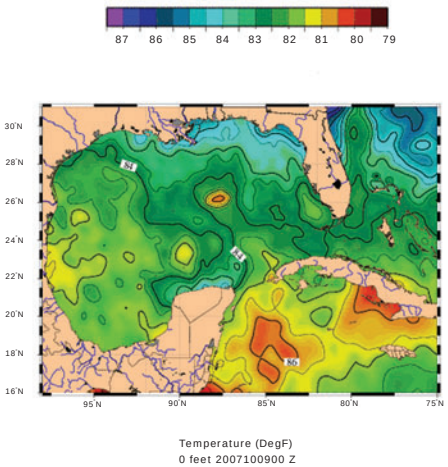


UNCLASSIFIED: MODAS Sea Temperature at Sea Surface

Operational Products generated on NAVO MSRC systems by METOC Operational Forecasting Groups. (L-R) Navy Coastal Ocean Model (NCOM) 36-hour current and speed forecast, Gulf of Mexico; 1/32 degree resolution Global Navy Layered Ocean Model (Global NLOM) sea surface height and surface current forecast, Hawaiian Islands; and Modular Ocean Data Assimilation System (MODAS) product: sea temperature at sea surface, Gulf of Mexico.

periods to accommodate the METOC group's oceanographic support of a series of exercises being conducted by the Navy fleet in conjunction with resources and service members from the Army, Air Force, Marine Corps, and Coast Guard.

Valiant Shield 07, as the eight-day Pacific exercise is known, required the uninterrupted delivery of forecast products from the NAVOCEANO operational team. These oceanographic products were delivered to the Naval Oceanography Antisubmarine Warfare (ASW) Teams (NOATs), who in turn used these products to provide recommendations on unit and ASW sensor deployments.

To assist in this effort the NAVO MSRC put its team on high alert throughout the exercise for swift response should any problems have arisen with the HPC systems. The overall teamwork between the MSRC and the local METOC operational community during such exercises helps condition both teams for any possible emergency military exercises as well.

The Navy METOC community and the Navy's survey fleet are sometimes called upon to provide ocean forecasting, sonar sea-floor mapping, and pinger location assistance in non-military recovery and salvaging efforts.

A previous effort in which operational forecasts were used in the December 2004 Indonesian tsunami rescue and recovery efforts was detailed in the Spring 2005 issue of the Navigator. Most recently the Indonesian government requested the Navy's assistance in locating the wreckage of Adam Air Flight KI 574 which went missing off the coast of West Sulawesi, Indonesia, on January 1, 2007.

The NAVOCEANO survey ship USNS *Mary Sears* traveled to the area and on January 9 joined the search effort team comprised of the National Transportation Safety Board (NTSB) and the Indonesian Search and Rescue Command Center (SAR).

The exact location of the lost plane was unknown. When a piece of wreckage washed up on the beach January 10, the NAVOCEANO ocean forecasting team was asked to project from where it may have come. Using surface currents from the NCOM model run daily on MSRC, a 10-day hindcast suggested where the plane went down. By using a towed pinger locator unit, the crew aboard the *Mary Sears* was able to locate the downed aircraft's pinger signal very near where NCOM said it would be.

This finding along with operational hydrographic forecasts and side-scan sonar charting of nearly three nautical miles of sea floor resulted in the *Mary Sears* crew locating the wreckage of the Boeing 737 and the flight data and cockpit voice recorders within several days of arriving on scene.

As always, the NAVO MSRC is committed to supporting the warfighter—both in support of the DoD HPCMP community and the day-to-day operations of the nation's military forces.

NAVOCEANO has technical control of six 329-foot-long, 5,000-ton T-AGS 60 class ships and one hydrographic ship designed to provide multipurpose oceanographic capabilities in coastal and deep-ocean areas. These include physical, chemical, and biological oceanography; multidiscipline environmental investigations; ocean engineering and marine acoustics; marine geology and geophysics; and bathymetric surveying.

Advance Reservation Service Available on KRAKEN

Christine Cuicchi, Computational Science and Applications Lead, NAVO MSRC

As part of a High Performance Computing Modernization Program (HPCMP) directive to provide interactive and real-time High Performance Computing (HPC) system access to the Department of Defense (DoD) user base on an as-needed basis, the NAVO MSRC will implement advanced reservations on the P4+ system, KRAKEN. This capability, which was available previously on the Army Research Laboratory's (ARL) Intel Xeon cluster POWELL, will also be offered on the ARL Linux Networx system, JVN.

This advance reservations system will allow users to request a specific run time in which to run interactive jobs, real-time simulations, or batch jobs. The reservation system being developed at press time will allow the user to authenticate on a front-end website via kerberos. First time users will be directed to request an account on the online reservation portal. After establishing an online reservation portal account, a user may request a number of whole nodes for a user-specified amount of time delineated in one-hour increments. In addition, users will be able to specify which project they would like to use.

When a reservation request is made, the user will receive an email containing the Load Sharing Facility (LSF) reservation identification number for their job, the nodes to which they have access, and the time of the reservation. This reservation identification number must be used to submit batch jobs in the following manner:

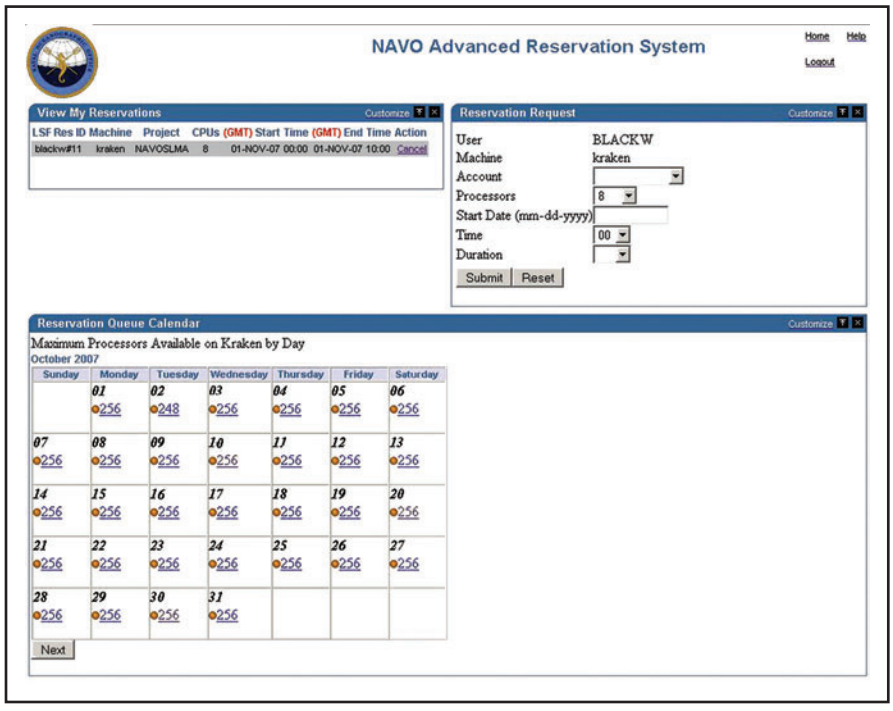
bsub -U reservation_id ..... < script

Users who wish to run interactive LSF jobs should submit them at the beginning of the reservation. Running the bsub command will allows users to see a list of reservations as well.

All reservations will begin at the time the user requests. Users will have the ability to cancel their reservations up to 30 minutes before the reservation start time. If the reservation is not cancelled, system utilization will be charged for these nodes regardless of how, or if, the nodes are used.

The initial deployment will allow for reservations on 256 processors (32 nodes) and will likely increase to 512 processors once the stability of the process has been established. The NAVO MSRC will continually monitor the need for this advance reservation capability and make adjustments as necessary.

Implementation and monitoring of the advance reservations system is courtesy of team members Grant Black, Patrick Thompson, and Lee Whatley, all of Lockheed Martin Mission Services (LMMS). For more information on how to schedule an advance reservation, please visit the NAVO MSRC website at http://www.navo.hpc.mil.



Screen shot of the NAVO Advance Reservation System.

COMPUTATIONAL CHEM
THE ATMOSPHE
TOXIC INDUSTRIAL C

Steven W. Bunte, Margaret M. Hurley, DeCarlos E. Taylor
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Melbourne, FL 32940

ISTRY MODELING OF
RIC FATE OF
COMPOUNDS (TICs)

Predicting the atmospheric fate of Toxic Industrial Compounds (TICs) is a critical component of the Department of Defense (DoD) chemical/biological defense programs as well as national security. Typically, Transport and Dispersion (T&D) models (e.g., Second-order Closure Integrated PUFF Model (SCIPUFF) or the recently parallelized ChemCODE/ChemCONC) that include atmospheric chemistry are used to generate such predictions. However, much of the critical kinetic data (i.e., rate constants, k(T)) needed for such modeling does not exist and is both difficult and expensive to obtain experimentally. Our unique approach to obtaining the all important k(T) is to use state-of-the-art computational quantum chemistry/chemical dynamics models to compute k(T), which can then be directly input into atmospheric chemistry modules.

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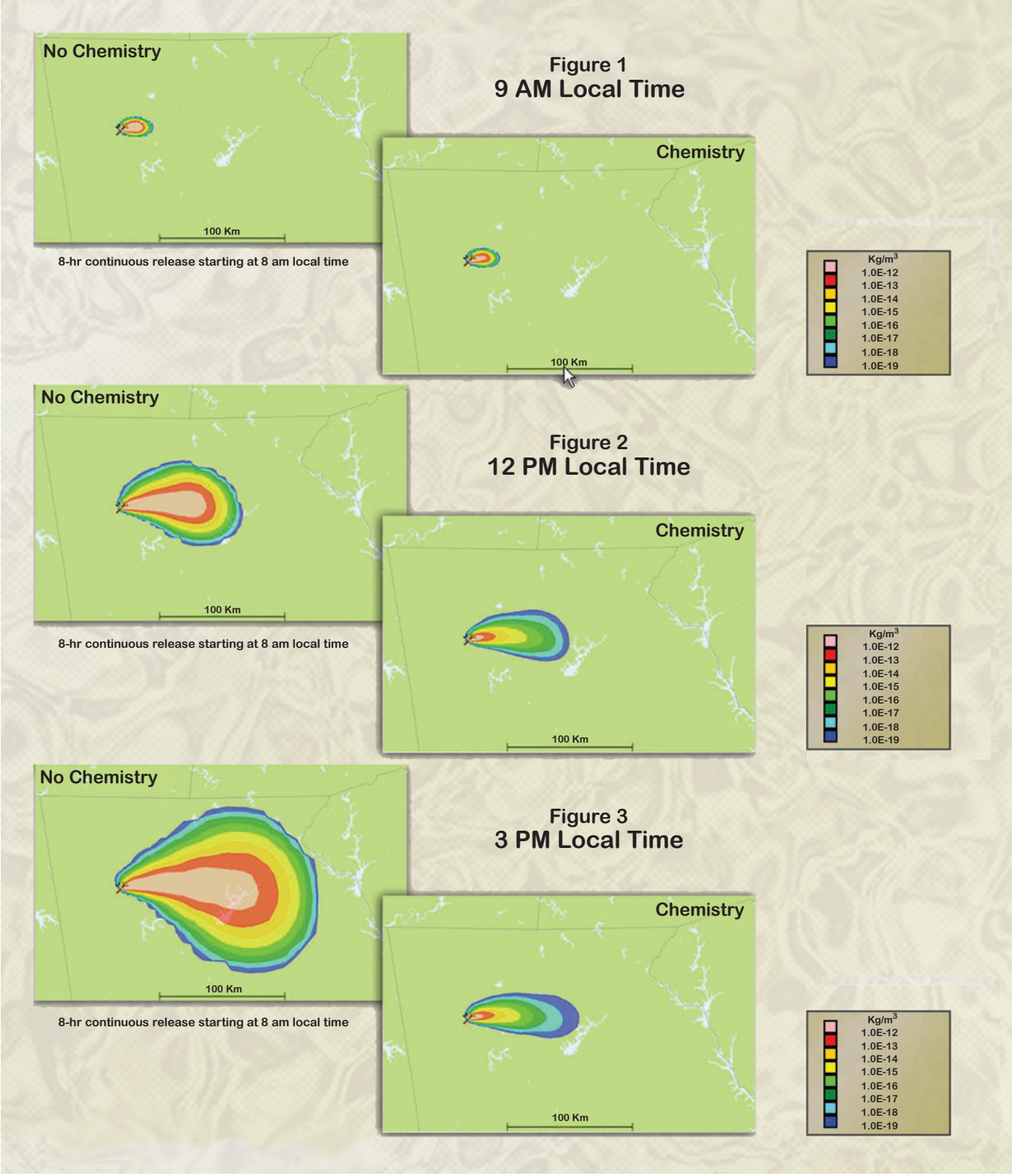

Figure 1. Plume model showing the contamination zone at 9am following the release of 2-methylpropane at 8am.

Figure 2. Plume model showing the contamination zone at noon following the release of 2-methylpropane at 8am.

Figure 3. Plume model showing the contamination zone at 3pm following the release of 2-methylpropane at 8am.

This innovation has resulted in an improved ability to model the fate of TICs in the atmosphere, resulting in more realistic representations of contamination zones. Such T&D methods can be used not only to predict the changing health threat in both urban and battlefield environments, but can also predict the nature of the resulting by-products.

This information, in turn, would be valuable in programming advanced sensors to warn of the release of a toxic compound even if the material has degraded by the time it reached the detection array. In addition, the results of these calculations can also be used to make a more scientifically defensible selection of simulants for challenging detectors, as well as assisting in the evaluation of both individual and collective protection systems.

These calculations could also be used to provide a sound theoretical underpinning to the development of physical properties data, which is critical for choosing the proper simulant for use in synthesis, fate, and decontamination studies, as well as in the assessment of new potential threat agents and the selection of improved decontamination concepts.

Figures 1, 2, and 3 each demonstrate the importance of including finite chemistry in Transport and Dispersion (T&D) models. Each figure is a snapshot in time showing the plume following the release of 2-methylpropane at 8 a.m.

The simulation incorporates realistic meteorological data and assumes a uniform release of the material. The figures each include two plots: one with the chemistry turned "off" and the other with chemistry turned "on." The color contours within each plume are computed concentrations of the parent compound.

In Figure 1, both plumes are similar in shape, aerial coverage, and concentration. Three hours later, as shown in Figure 2, the shape of the plumes, the aerial coverage, and the concentrations of 2-methylpropane are very different. This is primarily due to an increase in the sun angle, which results in a higher concentration of hydroxyl (OH) in the atmosphere. Finally, Figure 3 shows the plume 6 hours after release and 3 hours later than the plume shown in Figure 2.

The aerial coverage of the two plumes in Figure 3 is radically different. This series of snapshots underscore the importance of including accurate chemistry into the T&D models so that a realistic representation of the contamination zone can be predicted.

Accurate rate constants can be calculated using a combination Quantum Chemistry (QC)/Chemical Dynamics (CD) approach. The QC method is computationally intensive as it requires the use of high level ab initio quantum chemistry to calculate accurate structures of the TICs at the various important stationary points along the minimum energy path that connects reactants to products.

For the QC work, we use the ACESIII quantum chemistry package. ACESIII is the parallel version (developed under Common High Performance Computing Software Initiative (CHSSI) funding, project CBD-03) of the ACESII program, which itself was developed over the last 20-plus years under support from the Air Force Office of Scientific Research (AFOSR),

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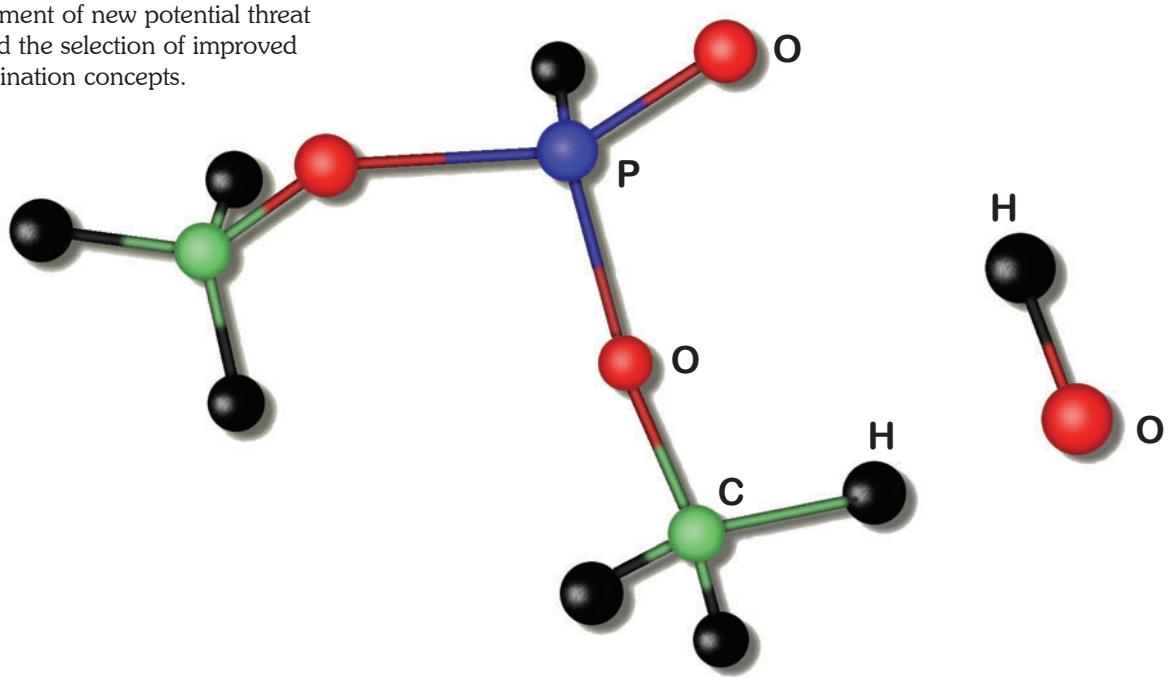

Figure 4. Representative Transition State for the Reaction of DMHP + OH.

Office of Naval Research (ONR), and Army Research Office (ARO).[1]

The ACESIII is a general QC package focusing on many body methods (i.e., finite-order Many Body Perturbation Theory (MBPT) and infinite order Coupled Cluster (CC) methods) and is used to compute molecular structures, energies, vibrational spectra, electronic spectra, magnetic properties, polarizabilities, etc.

The ACES program package was developed by Professor Rodney Bartlett and co-workers at the Quantum Theory Project of the University of Florida. The QC information is then input into a recently developed Semi-Classical Flux-Flux Autocorrelation Function (SCFFAF) chemical dynamics code, which computes the k(T) of the reaction under investigation over a wide temperature range. Details of this methodology can be found in K. Runge and M. G. Cory and R. J. Bartlett, "The Calculation of Thermal Rate Constants for Gas Phase Reactions: A Quasi-Classical Flux-Flux Autocorrelation function."[2]

The Reaction of Dimethyl Phosphonate (DMHP) + Hydroxyl Radical (OH)

When released into the troposphere, Dimethyl Phosphonate (DMHP) will degrade, for example, by reacting with OH radicals. The products of this hydrogen abstraction reaction are a radical DMHP species and water. Our calculations found four transition states that are accessible at ambient temperatures and are thus the major contributors to the total rate.

Figure 4 shows a representative transition state for the abstraction of a hydrogen atom from one of the methyl groups on DMHP; this transition state is also the major contributor to the total rate. Figure 5 shows the computed temperature dependent rate constants for each of these mechanisms, as well as the total rate constant, which is simply the sum of the individual rate constants. Our calculated total rate constant agrees quite favorably with the experimental rates measured by Atkinson.[3] Note that each of the experimental data points is an individual measurement at a single temperature, whereas our calculations give the full temperature dependent rate.

Conclusions

In this work, we have used a combination of quantum chemistry and chemical dynamics to theoretically predict the temperature dependent rates for the abstraction of hydrogen atoms by OH radicals from dimethyl phosphonate. These computed rate constants will now be used as input into atmospheric chemistry modules within DoD T&D models, such as SCIPUFF and ChemCODE/ChemCONC. The addition of finite chemistry will result in the improved ability of the models to handle the fate and interaction of TICs in the atmosphere, resulting in a more realistic representation of the contamination zone.

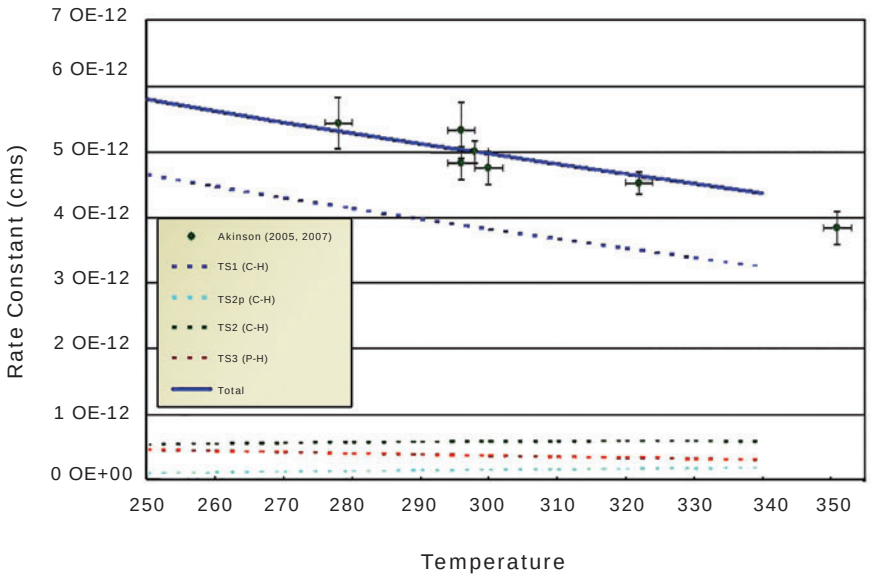

Figure 5. Temperature Dependent Rate Constants for the Reaction of DMHP + OH.

References

1. DoD High Performance Computing Modernization Program Office (HPCMPO) Common High Performance Computing Software Support Initiative (CHSSI) Program (Project CBD-03)
2. Runge, K., M.G. Cory, and R.J. Bartlett. "The Calculation of Thermal Rate Constants for Gas Phase Reactions: A Semiclassical Flux-Flux Autocorrelation Function (SCFFAF) Approach." Journal of Chemical Physics 114(2001): 141-5148.
3. Aschmann, S.M., E.C. Tuazon, and R. Atkinson. "Atmospheric Chemistry of Dimethyl Phosphonate, Dimethyl Methylphosphonate, and Dimethyl Ethylphosphonate." Journal of Physical Chemistry A 109 (2005): 11828-11836, and unpublished results.

Setting Standards in the Technology Insertion Process

Christine Cuicchi, Computational Science and Applications Lead, NAVO MSRC

The one constant in the world of High Performance Computing (HPC) is change. As computing technology grows ever more sophisticated, greater computing power becomes available. To keep this power harnessed for use by Department of Defense (DoD) users, the High Performance Computing Modernization Program (HPCMP) administers the annual Technical Insertion (TI) process.

The TI process encompasses staff members of the four HPC Major Shared Resource Centers (MSRCs), the Shared Resource Centers (SRCs), and advisors from selected support contract companies. These individuals are selected to tap into their HPC and User Support expertise to ensure that the DoD's annual procurement of HPC systems ($40-60 million worth in TI-08) is used to provide the best environment and technology for users now and in the future.

To streamline efforts, participants are divided into three teams: Usability, Performance (which evaluate vendor proposals), and Document preparation (which prepares TI Request for Quotes (RFQs)).

Since 2000, NAVO MSRC staff and HPC resources have been intimately involved in all aspects of the intricate HPCMP TI process.

Benchmarking

As the TI process has matured over the past seven years, the Performance Team has created and enhanced a TI application benchmark suite, a synthetic benchmark suite, and a performance prediction system. As a vendor submits an application, the Team evaluates a vendor's performance against these pre-established benchmarks based on the vendor's ability to compile their application and then runs it against the benchmarks within a specified speedup over the standard DoD system's TI application run times. The TI-08 application suite consists of applications chosen to represent the overall requirements of the DoD HPCMP user base:

- AERO
- COBALT
- CTH
- GAMESS
- HYCOM
- OOCORE
- AMR
- ICEPIC
- LAMMPS
- OVERFLOW-2
- WRF

Vendors are also evaluated on system performance metrics gathered via both the synthetic benchmarks and the performance prediction system developed at the San Diego Supercomputing Center.

NAVO MSRC staff member Christine Cuicchi and Productivity Enhancement Technology Transfer (PET) on-site Dr. John Cazes (Texas Advanced Computing Center (TACC)) have served on the Performance Team since the TI-02 and TI-05 efforts, respectively. For the TI-08 effort, Dr. Cazes remains on this team while Ms. Cuicchi has joined the Usability Team.

The Usability Team reviews vendor proposals for robustness and ease of use based on a number of criteria, including the availability of key commercial software packages, system utilities, and system characteristics that facilitate integration, operation, maintenance, and upgrades. Past Usability Team members from the NAVO MSRC have included Dr. Cazes (TACC), Ed Farrar (Lockheed Martin Space Operations (LMSO)), Lee Whatley (Lockheed Martin Mississippi Space & Technology Center (LMMS)), and Dave Cole (NAVO MSRC), who led the team for the TI-06 process. Mr. Whatley is once again serving on the Usability Team for the current TI-08 process, and Mr. Cole has been serving as the Document Preparation Team lead since TI-07.

NAVO MSRC TI Benchmarking

NAVO MSRC HPC systems have also been an important part of the TI-XX process over the past several years. Each year, one production system in the HPCMP is selected to be the DoD standard performance system, against which vendor proposals and performances will be evaluated. In TI-03, the NAVO MSRC 1024 processor IBM Power3 system HABU was chosen to be the DoD standard system. HABU served as the standard system until TI-05, when it was replaced by the NAVO MSRC TI-04 acquisition system KRAKEN – an IBM Power4+ 2944 processor machine. In 2007, the Engineer Research and Development Center (ERDC) MSRC Cray XT4, SAPPHIRE, was selected by the Performance Team to be the TI-08 standard system, thus ending the reign of NAVO MSRC systems as

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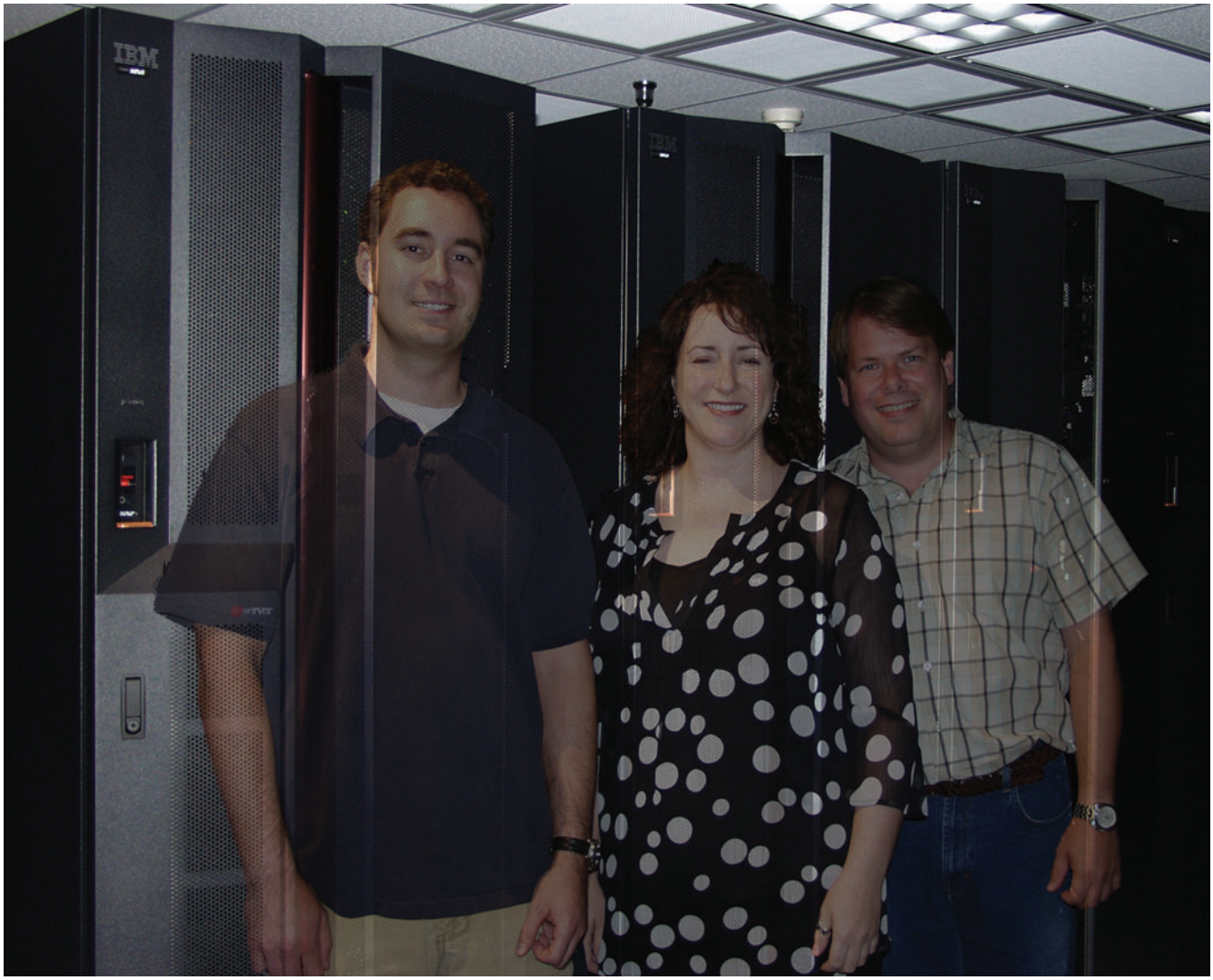
representative of the DoDs required performance ability. However, HABU remains the HPCMP's best example of a balanced system—production systems and proposed systems are still compared with the performance of the 1024 processor HABU.

Another important component of the NAVO MSRC's support of the TI process has been support of the benchmarking efforts, both to garner standard system runtimes as well as benchmarking the performance of other production HPC systems installed at the NAVO MSRC. In the initial years of the TI process, the staff at each MSRC was responsible for running the entire applications suite on each production HPC system at their site. This task has since fallen under the auspices of the ERDC MSRC's Computational Science and Applications (CS&E) Team and the Performance Modeling and Characterization (PMaC) laboratory at the San Diego Supercomputing Center (SDSC). NAVO MSRC staff continues to work closely with these teams to ensure fast turnaround and proper support to keep within the tight TI schedule.

Conclusion

The NAVO MSRC is proud to have been a substantial part of the Technology Insertion process and looks forward to continuing to provide technical expertise and HPC system support in assisting the HPCMP in selecting the most effective and efficient HPC systems for its users.



Three members of the NAVO MSRC TI 08 team: (L-R) Lee Whatley (Lockheed Martin Mississippi Space & Technology Center (LMMS), Christine Cuicchi (Computational Science and Applications Lead, NAVO MSRC), and Dr. John Cazes (Texas Advanced Computing Center (TACC)).

Navigator Tools and Tips

LSF Top 5 FAQs

Sheila Carbonette, NAVO MSRC User Support

The Computing Load Sharing Facility (LSF) by Platform Computing is the batch scheduler currently used on the NAVO MSRC IBM systems KRAKEN, PASCAL, and ROMULUS. This issue of Tips 'n Tricks is designed to provide answers to some of our user's most frequent questions.

Q. Where can I learn how to use LSF?

A. An introductory guide can be found on the NAVO MSRC website. The URL of the LSF introduction is: http://www.navo.hpc.mil/lsf_guide.html

The guide provides an overview of LSF, a comparison of LoadLeveler and LSF commands and example scripts.

Q. How do I make one batch job wait for another to complete?

A. LSF handles this through the use of job dependencies with the "bsub" command wait option, "-w". The wait option allows you to specify the condition which you wish to wait for before starting the job.
An example batch script that uses the wait option to start the second job at the completion of the first job follows:

```
kraken% cat job01
#BSUB -P NAVOSLMA
#BSUB -o %J.log
#BSUB -e %J.err
#BSUB -J job01
#BSUB -N
#BSUB -W 1:30
#BSUB -R "span[ptile=8]"
#BSUB -n 8
#BSUB -q standard
#
# RUN PARALLEL EXECUTABLE
./mpirun.lsf mpijob.exe
#
# SUBMIT SECOND JOB
bsub < job02
#
# END OF job01 SCRIPT
```

```
kraken% cat job02
#BSUB -P NAVOSLMA
#BSUB -o %J.log
#BSUB -e %J.err
#BSUB -J job02
#BSUB -w 'done("job01")'
#BSUB -N
#BSUB -W 0:30
#BSUB -R "span[ptile=8]"
#BSUB -n 8
#BSUB -q standard
#
# RUN PARALLEL EXECUTABLE
./mpirun.lsf mpijob2.exe
#
# END OF job02 SCRIPT
```

Additional information on the wait option can be found in the bsub main page.

Q. My parallel batch job failed with the following message:

```
"Cannot find enough ntbl windows on sni0.
Exiting ..."
```

What does this error mean?

A. This error can mean a couple of things. The easiest to check first is the quota on your home directory. If you have exceeded your quota, or are near exceeding your quota, then LSF can't write required host files to your home directory. The following is an example listing of the file names:

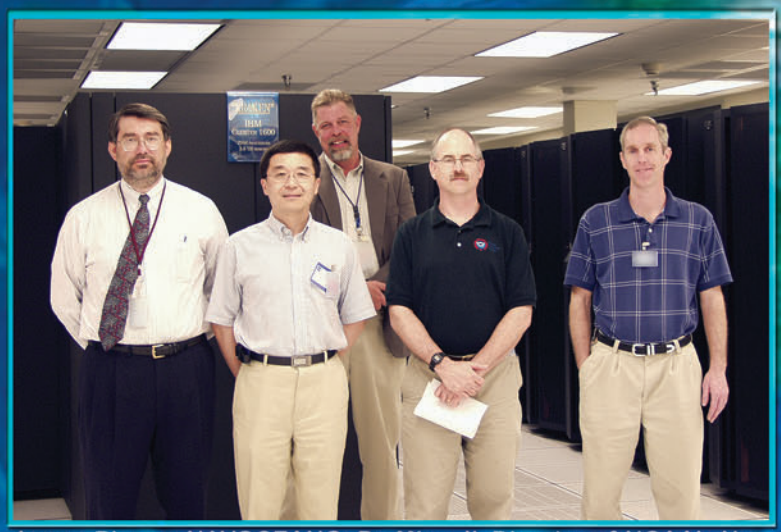
```
kraken% ls -al .sni* .windows* .all.hosts.* .host.
list.*
-rw-rw----  1 shecar NAVOSLMA    10483 Sep
23 13:57 .sni0.289394
-rw-rw----  1 shecar NAVOSLMA    10483 Sep
23 13:57 .sni0.289394.1
-rw-rw----  1 shecar NAVOSLMA    10563 Sep
23 13:57 .sni1.289394
```

Continued Page 22

The Porthole

Tom Dunn, NAVO MSRC Director; CAPT Kusters, Prospective Commanding Officer of FNMOC; Dave Cole, Christine Cuicchi, NAVO MSRC.

John Choplinsky, Deputy Comptroller, U.S. Fleet Forces Command



James Rigney, NAVOCEANO; Dr. Ming Ji, Director of NOAA's National Environmental Prediction Center's Ocean Prediction Center; Pete Gruzinskas, NAVO MSRC; Joseph Sienkeiwicz and Robert Daniels, NCEP OPC.

Basic Oceanography Accession Training (BOAT) class tour the MSRC with Christine Cuicchi, NAVO MSRC.

Tom Dunn, NAVO MSRC Director and John Dupuis, NAVO MSRC, brief visitors from Information Management Resources, Incorporated (IMRI)

CAPT Robert E. Kiser, CNMOC; CAPT Brian B. Brown, NAVOCEANO; CAPT David Titley, CNMOC; CAPT John D. Cousins, NAVOCEANO; RDML Timothy McGee, CNMOC; RADM David Gove, Oceanographer of the Navy; Tom Dunn, Director NAVO MSRC; Ed Gough, Deputy/Technical Director CNMOC; John Lever, CNMOC; CAPT Jeffrey Best, OPNAV.

Dave Cole, NAVO MSRC; Tom Dunn, NAVO MSRC Director; and Ed Gough, Deputy/Technical Director CNMOC brief Scott McNealy, Chairman of Sun Microsystems (center) and party at the NAVO Major Shared Resource Center

Industry Education Partnerships Workshop sponsored by Mississippi State University and the National Science Foundation

```
-rw-rw----  1 shecar NAVOSLMA   10563 Sep
23 13:57 .sni1.289394.1
-rw-rw----  1 shecar NAVOSLMA   10214 Sep
23 13:57 .windows.289394.1
-rw-rw----  1 shecar NAVOSLMA   682 Sep 23
13:57 .all.hosts.289394
-rw-rw----  1 shecar NAVOSLMA   5456 Sep
23 13:57 .host.list.289394
```

You can check your quota with the /site/bin/quota command.

```
kraken% /site/bin/quota
                              Block Limits
Filesystem type      KB     quota  limit  in_
doubt  grace
gpfs_hm     USR   517364  512000 524288
2054        expired
```

(Note: The output from the quota command has another section for “File Limits” that was omitted in this example.)

This second reason can be that your job is not getting all of the adapter windows available on a given node. To ensure your job does not start until all of the adapter windows are available on a node, the following resource requirement can be added to your batch script:

For KRAKEN:

```
#BSUB -R 'rusage[ntbl_windows=16]span[ptile=8]'
```

For BABBAGE:

```
#BSUB -R 'rusage[ntbl_windows=32]span[ptile=16]'
```

Another useful command to get this information as well as your allocation usage is the "show_usage" command.

For example:

```
/kraken% /site/bin/show_usage
```

Q. When I try to submit a job, I get the error message:

```
"shecar is not authorized to use project
NRLSS03755018 .
```

How do I find out my project name?

A. The NAVO MSRC uses an eight-character naming convention for projects instead of the 13 character full sub-project identifier. The NAVO MSRC eight-character identifier is composed of the five-character Organization ID and the three-character allocation number assigned by the Service/Agency Approval Authority (S/AAA).

For example: Full Subproject Identifier: NRLSS03755018
NAVO MSRC Project/Group Identifier: NRLSS018

The easiest way to determine the project name, is to type the unix command, groups. At the MSRC, the project identifier is the same as the group name. For example:

```
kraken% groups shecar
  shecar: NRLSS018
```

Another useful command to get this information as well as your current allocation is the **show_usage** command. For example:

```
kraken% /site/bin/show_usage

Date      Time      System    Account
10/01/07 12:16:13    kraken  NRLSS008
     Allocated     20000.00
     Used          0.00
     Balance       20000.00
     Percent       0.00 used
```

Q: Where can I go to get more help?

A. The questions addressed in this article and others are found in the Frequently Asked Questions (FAQ) web page available at the following URL: http://www.navo.hpc.mil/user_tips.html

This FAQ page also includes information and links to help you get oriented with the different High Performance Computing (HPC) systems and the Archive servers. If you can't find an answer to your question on this page, you can always call the Consolidated Customer Assistance Center (CCAC) or NAVO MSRC User Support for assistance:

The Consolidated Customer Assistance Center (CCAC) is available 0700–2200 (Central Time), Monday–Friday for issues of an unclassified nature:

- Help Desk toll free number: 1-877-CCAC-039 or 1-877-222-2039
- Help Desk email address: help@ccac.hpc.mil
- Website: http://www.ccac.hpc.mil

NAVO MSRC User Support is available 0800–1630 (Central Time), Monday–Friday, for issues of a classified nature:

- User Support toll free number: 1-800-993-7677
- Help Desk E-mail: msrchelp@navo.hpc.mil
- Website: http://www.navo.hpc.mil

Coming Events

Annual Computer Security Applications Conference
December 10-14, 2007
Miami Beach, Florida, USA
http://www.acsac.org/

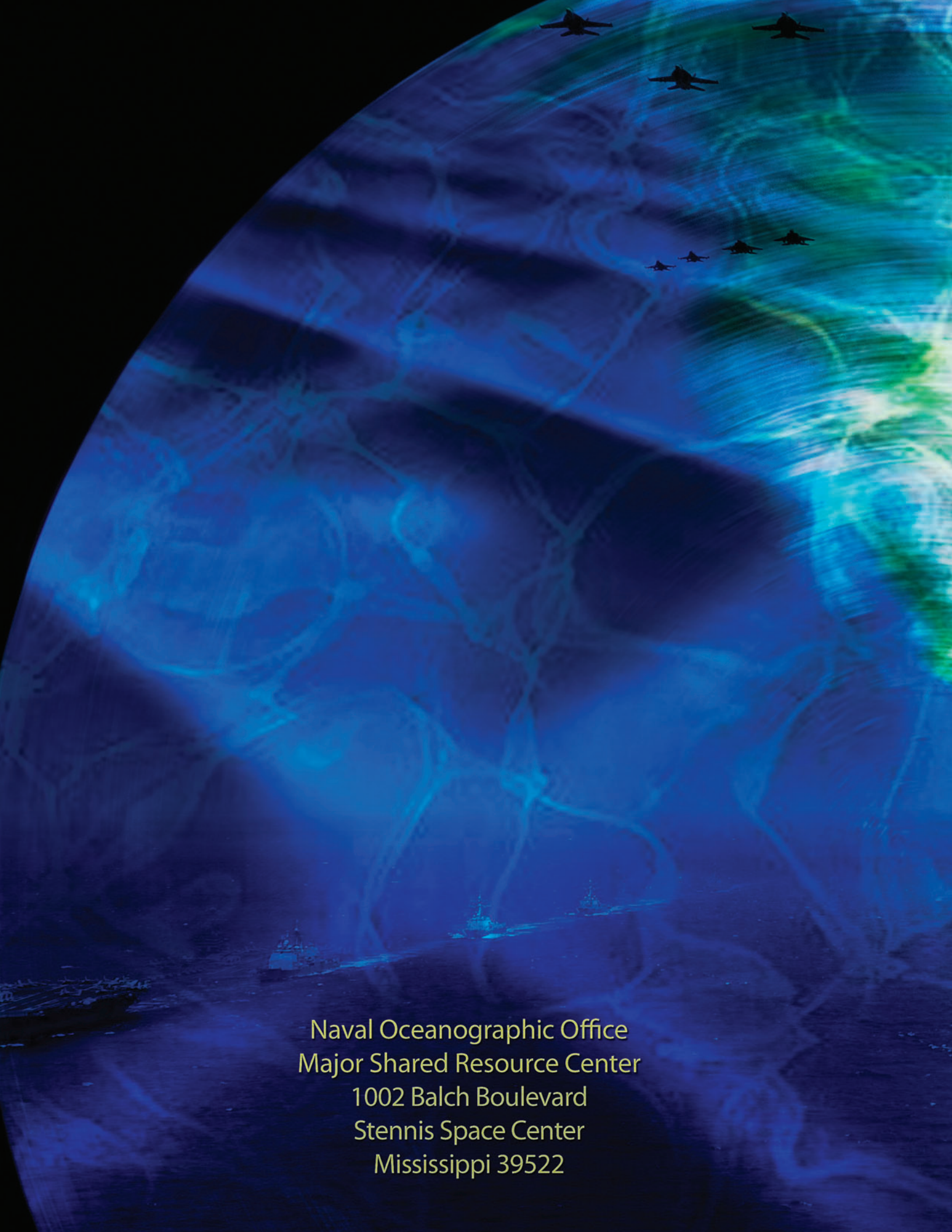
HiPC 2007
International Conference on High Performance Computing
December 18-21, 2007
Goa, India,
http://www.hipc.org/

PPoPP'08
13th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming
February 16-20, 2008
Salt Lake City, UT
http://research.ihost.com/ppopp08/

HPCA'08
14th International Symposium on High-Performance Computer Architecture
February 16-20, 2008
Salt Lake City, UT
http://www.cs.utah.edu/hpca08/

IPDPS 2008
The 22nd IEEE International Parallel and Distributed Processing Symposium
April 14-18, 2008.
Miami, FL
http://www.ipdps.org/

ISC
International Supercomputing Conference
June 17-20, 2008
Dresden, Germany
http://www.supercomp.de/isc08/index.php5



Naval Oceanographic Office
Major Shared Resource Center
1002 Balch Boulevard
Stennis Space Center
Mississippi 39522