Selected NERSC Initiative for Scientific Exploration (NISE) Research Summaries: 2010

Project: Decadal Predictability in CCSM4
PI: Haiyan Teng and Grant Branstator, NCAR
NERSC Repo: mp9
NISE hours awarded: 1.6 M

With the NISE award, we have carried out two 25-member CCSM4 ensemble experiments with perturbed initial condition. The ensemble experiment has led to findings that should influence the direction of major ongoing international climate research efforts. In order to provide society with the most accurate possible estimates of climate in the coming decades, the scientific community is devoting much effort to initializing some forecasts in the next IPCC assessment report with estimates of the current state of the climate system. The results the decadal predictability project suggest that a quantification of the inherent predictability limits of each model used in these projections is needed so that forecast design and interpretation can properly take into account these limitations.

Publications and Presentations:
Branstator, G. and H. Teng, 2011, Two Limits of decadal predictability in two generations of CCSM, 23rd Conference on Climate Variability and Change, Seattle, January 2011

Tribbia, J. et al. 2011, Journal of Climate, in preparation.

Projects (2): Developing an Ocean-Atmosphere Reanalysis for Climate Applications (OARCA) for the Period 1850 to the Present; and Surface Input Reanalysis for Climate Applications 1850 – 2011
Investigators: Gilbert Compo, Jeffrey Whitaker, Benjamin Giese, and Prashant Sardeshmukh (University of Colorado)
NERSC Repo: mp958
NISE hours awarded: 2M

These NISE efforts build on the 20th Century Reanalysis Project (20CR) generated at NERSC. 20CR produced the first set of global weather maps from the surface of the earth to the jet-stream level extending back to 1871. The 20CR is being used to address issues in climate variability and change, such as climate extremes, hurricanes, droughts, and floods. While extremely useful, there are several avenues for improvement. Two are being addressed using NISE hours. We have started an investigation of the importance of a coupled ocean-atmosphere assimilation system

for representing historical extreme weather and climate events. We have found that using 8 of the member of the 20CR ensemble to provide boundary forcing for an ocean assimilation, we are getting a non-linear effect whereby the mean of the individual tates is not as large an amplitude determined as using the 20CR ensemble mean. With additional runs, we will be able to determine if this is a sampling issue and all 56 of the ensemble members need to be used. To improve the atmospheric data assimilation, we have made tests of the use of additional surface observation types beyond surface pressure observations. In particular, we have examined the impact of near-surface winds. While wind assimilation improves the representation of the atmosphere in the tropics, it degrades the mid and high latitudes. Causes for this will be under investigation in our 2011 NISE project.

Publications

Brönnimann, S., G.P. Compo, R. Spadin, R. Allan, and W. Adam, 2011: Early ship-based upper-air data and comparison with the Twentieth Century Reanalysis. Clim. Past, 7, 265-276, doi:10.5194/cp-7-265-2011.

Brönnimann, S., and G.P. Compo, 2011: Ozone highs and associated flow features in the first half of the twentieth century in different data sets. Meteorol. Zeit., in press.

Compo, G.P., J.S. Whitaker, P.D. Sardeshmukh, N. Matsui, R.J. Allan, X. Yin, B.E. Gleason, R.S. Vose, G. Rutledge, P. Bessemoulin, S. Brönnimann, M. Brunet, R.I. Crouthamel, A.N. Grant, P.Y. Groisman, P.D. Jones, M. Kruk, A.C. Kruger, G.J. Marshall, M. Maugeri, H.Y. Mok, Ø. Nordli, T.F. Ross, R.M. Trigo, X.L. Wang, S.D. Woodruff, and S.J. Worley, 2011: The Twentieth Century Reanalysis Project. Quarterly J. Roy. Met. Soc., 137, 1-28, doi: 10.1002/qj.776

Giese B.S., G.P. Compo, N.C. Slowey, P.D. Sardeshmukh, J.A. Carton, S. Ray, and J.S. Whitaker, 2010:The 1918/1919 El Niño. Bull. Amer. Meteor. Soc., 91, 177-183, doi: 10.1175/2009BAMS2903.

Recent Publications that use the data but for which the PI is not a co-author:

Baird, M.E., J.D. Everett, and I.M. Suthers, 2011: Analysis of southeast Australian zooplankton observations of 1938-1942 using synoptic oceanographic conditions. Deep Sea Res. II, 58:699-711 doi:10.1016/j.dsr2.2010.06.002.

Barriopedro D., E.M. Fischer, Luterbacher J., Trigo R.M., and R. García-Herrera, 2011: The Hot Summer of 2010: Redrawing the Temperature Record Map of Europe, Science, published online 17 March 2011, DOI:10.1126/science.1201224.

Bye, J., K. Fraedrich, E. Kirk, S. Schubert, and X. Zhu, 2011: Random walk lengths of about 30 years in global climate, Geophys. Res. Lett., 38, L05806, doi:10.1029/2010GL046333.

Cook, B.I, R. Seager, and R.L. Miller, 2010: Atmospheric circulation anomalies during two persistent north american droughts: 1932-1939 and 1948-1957. Clim. Dyn., in press, doi: 10.1007/s00382-010-0807-1.

Dole, R., M. Hoerling, J. Perlwitz, J. Eischeid, P. Pegion, T. Zhang, X.-W. Quan, T. Xu, and D. Murray, 2011: Geophys. Res. Lett., 38, L06702, doi:10.1029/2010GL046582.
Emanuel, K., 2010: Tropical Cyclone Activity Downscaled from NOAA-CIRES Reanalysis, 1908-1958. J. Adv. Model. Earth Syst., Vol. 2, Art. #1, 12 pp., doi:10.3894/JAMES.2010.2.1
Giese B.S., and S. Ray, 2011: El Niño variability in simple ocean data assimilation (SODA) 1871-2008.J. Geophys. Res.-Oceans., 116, C02024 doi:10.1029/2010JC006695.
Truchelut, R. E., and R. E. Hart, 2011: Quantifying the possible existence of undocumented Atlantic warm-core cyclones in NOAA/CIRES 20th Century Reanalysis Data, Geophys. Res. Lett., 38, L08811, doi:10.1029/2011GL046756.
Wood, K. R., and J.E. Overland, 2010: Early 20th century Arctic warming in retrospect, Int. J. of Climatol., 30, 1269-1279, doi: 10.1002/joc.1973.
Zhao, P., S. Yang, H. Wang, and Q. Zhang, 2011: Interdecadal relationships between the Asian-Pacific Oscillation and summer climate anomalies over Asian, North Pacific and North America during recent 100 years. J. Climate, in press. doi:10.1175/JCLI-D-11-00054.

Project: Light Propagation in Nanophotonics Structures Designed for High-Brightness Photocathodes
PI: Katherine Harkay, Karoly Nemeth and Joseph Zsolt Terdik , ANL
NERSC Repo: m878
NISE hours awarded: 1.3 M

We have continued working along the lines described in our recent Physical Review Letters paper (PRL 104, 046801 (2010)) to design and develop improved photocathodes. As our experimental collaborators were most interested in finding an improved replacement for the well established Cs2Te based photocathode material, we have conducted design and simulations on suitable improved alternative materials using our NISE resources and the Quantum Espresso code. We have screened several materials and finally converged to an other existing material that has nearly identical lattice parameters with Cs2Te, a very similar atomic distribution, a similar density of states, but it does not contain the health hazard material Te, and does not develop an oxide surface layer during operation of the photocathode under practical conditions. The calculations were carried out mostly by our student, J.Z. Terdik (University of Chicago). The suggested material is being synthesized by our experimental collaborators and will be tested in the coming months. We expect to publish a Physical Review B (or similar) paper from the theoretical findings soon. The potential to patent the suggested new photocathode material is also considered.

Project: Simulation of Elastic Properties and Deformation Behavior of Light-Weight Protection Materials Under High Pressure
PI: Wai-Yim Ching , University of Missouri, Kansas City

NERSC Repo: mp250
NISE hours awarded: 1.7 M

We received two previous NISE allocations. One project is for the DNA elasticity that constitutes the bulk part of the Ph.D. dissertation of a graduate student (Lei Liang). The work is a more in-depth study on her general computational research on biomaterials and biomolecular systems using NERSC resources [1, 2]. It turns out that this elasticity study on DNA is extremely demanding but exciting and requires 50-100 times more computational time than originally envisioned. This is due to the far more stretching steps of the two DNA models with improved convergence needed. We plan to complete the initial part of this study in a few months (after Hopper II trial period is over) and submit a comprehensive paper to a top peer-reviewed journal [3]. Some preliminary result on this project is show in Fig. 1 and Fig. 2. It shows an unexpected and puzzling discontinuity in the calculated total energies of the two DNA models (AT-10 and CG-10) under tensile strain at about 80% elongation. Detail analysis on the electronic structure revels that this could be due to the change in the H-bonding between base pairs at this particular elongated geometry which appears to be consistent with very limited experimental observations.

The second project of the NISE award is the simulation of elastic properties and deformation behavior of light-weight protection material under high pressure. This project went pretty well as expected using the uniaxial compression simulation on several 180-atom supercell models of boron carbide (B_4C) in the hexagonal lattice. The research accomplished under this project has been presented at several international symposia and conferences as invited talks and were well received. This work is now being drafted for publication [4] and no detailed description is enclosed in this short report unless specifically required by NERSC. No further simulation on B_4C is planned at this stage because we were unable to secure financial support from the US Department of Defense.

The above work on armor ceramics and other simulational studies [5, 6] under the regular ERCAP award prompted us to submit the current pending NISE application on the construction of multi-axial failure envelope in MAX phase compounds. Figure 3 shows the preliminary result with limited data points on the 192-atom supercell of the anisotropic layered compound Ti_3AlC_2. This result demonstrates the proof-of-the-concept of what we proposed to accomplish in this project which could lead to an entirely new approach in the computational studies of the mechanical properties of materials. We look forward to a favorable decision on our request.

Publications: (The following publications all acknowledge NERSC support)

[1]. Lei Liang, Paul Rulis and W.Y. Ching, "Mechanical properties, electronic structure and bonding of α- and β- tri-calcium phosphates with surface characterization", Acta Biomaterialia, 6, 3763-3771 (2010).

[2]. Lei Liang, Paul Rulis, L. Ouyang, and W.Y. Ching, "*Ab initio* investigation of H-bonding and network structure in bulk water", Phys. Rev. B 83, 024201-1-7 (2011) .

[3]. Lei Liang, Paul Rulis, L. Ouyang, and W.Y. Ching, "Ab initio study of elasticity of models of DNA", to be submitted to a peer reviewed journal.

[4] S. Aryal, Paul Rulis and W.Y. Ching, "Mechanism of amorphization in boron carbide (B_4C) under uniaxial compression", to be submitted to Phys. Rev. B.

[5]. W.Y. Ching, Paul Rulis[1] and A. Misra,"*Ab initio* elastic properties and tensile strength in hydroxyapatite crystal", Acta Biomaterialia, 5, 3067-3075 (2009).

[6].W.Y. Ching, Paul Rulis, Lizhi Ouyang, S. Aryal, and Anil Misra, "Theoretical study of the elasticity, of the mechanical, behavior, electronic structure, interatomic bonding, and dielectric function of an intergranular glassy film model in prismatic β-Si_3N_4", Phys. Rev. B 81, 214120-1-14. (2010).

[7]. Paul Rulis and W.Y. Ching, "Theoretical XANES spectra of Si-K, Si-L, N-K and O-K edges of a prismatic model of intergranular glassy films in ?-Si_3N_4", (Accepted by J. of Materials Science, 2011).

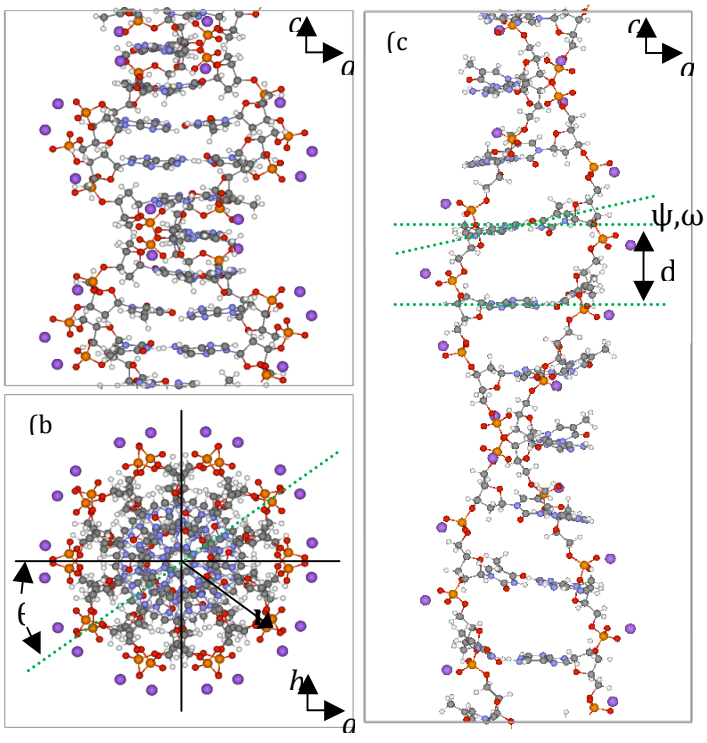

Figure 1. (a) The ball and stick model of the AT-10 DNA model with charge compensating Na counter ions. The model is periodic in the z-direction (vertical

axis) and contains a total of 660 atoms. (b) The same model as (a) viewed in the planer (x-y) direction. (c) The converged geometry of the model at near 80 % of elongation. The electronic structure and bonding at each stage of the elongation have been calculated and analyzed.

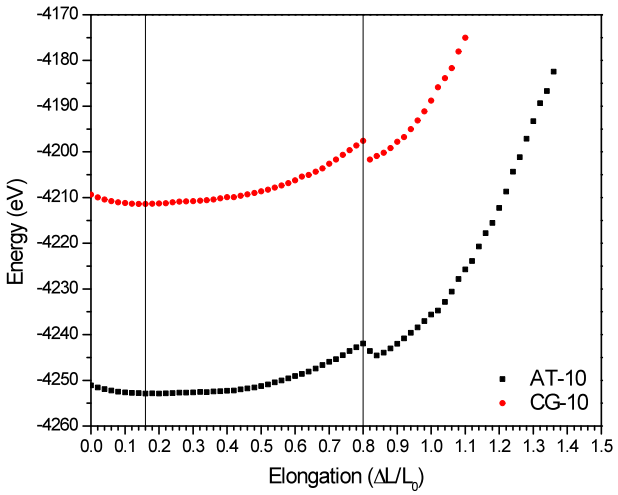

Figure 2. Total energy vs. the elongation of the two DNA models of Figure 1 showing an unexpected change in the curves at 80% elongation from the initial models.

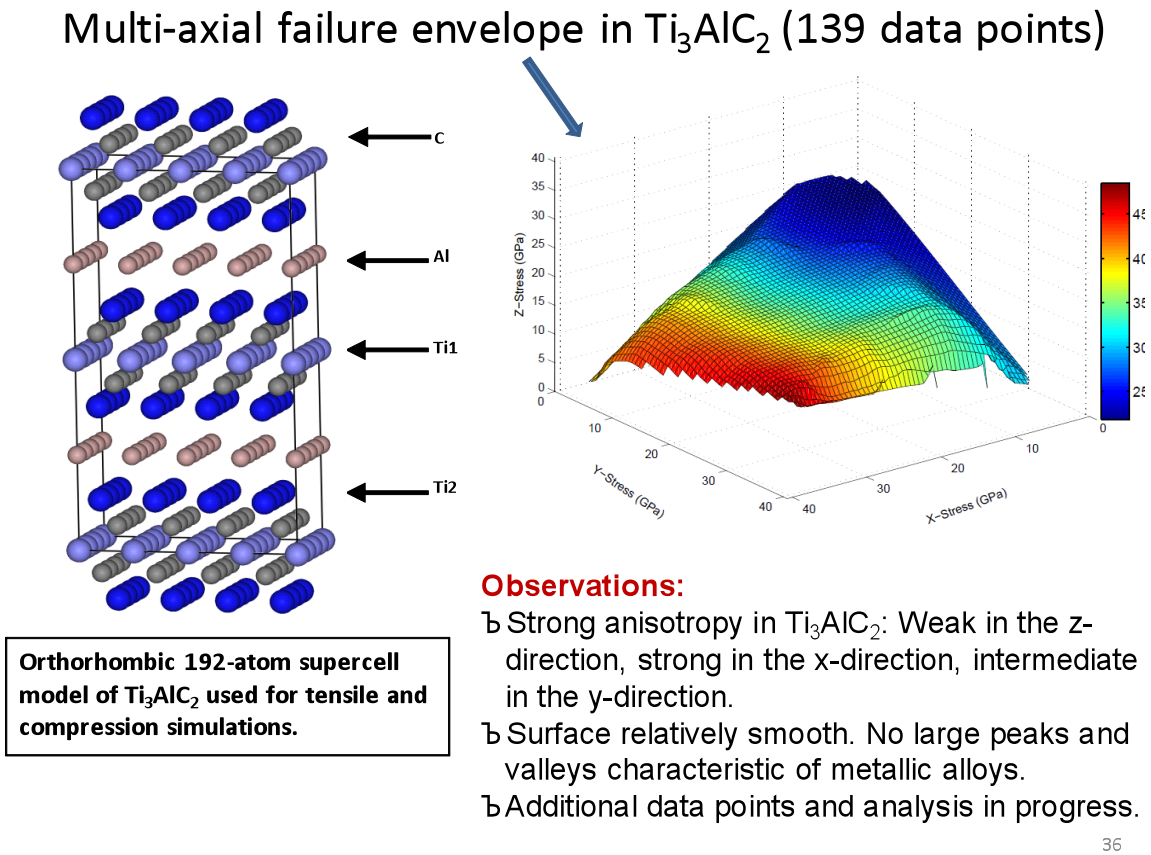

Figure 3. Preliminary result on the construction of a failure envelope for the MAX phase compound Ti_3AlC_2. Left panel: The 192-atom supercell of the crystal. Right panel: failure envelope based on 139 data points corresponding to tensile simulations in 139 directions.

Project: Modeling the Energy Flow in the Ozone Recombination Reaction
PI: Dmitri Babikov, Marquette University
NERSC Repo: m409
NISE hours awarded: 260,000

Using the "NERSC Initiative for Scientific Exploration" allocation of time award in 2010 we were able to carry out calculations of cross sections for the recombination reaction that forms ozone, namely for the energy transfer step of this reaction, which is the rate limiting step. In this process a metastable state of ozone (a scattering resonance) collides with the bath gas atom (Ar in our calculations). The ro-vibrational energy of ozone is transferred to the translational motion of Ar. We utilize the fact that the relative Ar + O3 collisional motion can be treated classically. The rotational motion of O3 can also be treated classically, because energy spacings between the rotational states are small, and because many rotational levels are

usually excited, even at low temperatures. The vibrational motion of O3, however, should be treated quantum mechanically in order to preserve zero-point energy, describe quantization of vibrational levels (including that of scattering resonances) and build symmetry constrains into the dynamics of collision.

Thus, in our approach the collisional Ar + O3 motion and the rotational motion of O3 are treated with classical trajectories. The vibrational motion of O3 is treated with time-dependent Schrödinger equation using the wave packet propagation technique. Quantum (vibrational) state of the system affects motion of its classical part (scattering and rotation) through the gradient of average potential, average rotational torque and average tensor of inertia using the mean field approach. In turn, classical part of the system affects dynamics of the quantum part through the potential energy term and the centrifugal potential term introduced into the Hamiltonian. The centrifugal potential energy is a function of internal vibrational coordinates, just like the potential energy surface. No rigid rotor (e.g., symmetric top) or any other kind of approximation is used. Instead, the centrifugal potential energy function is rigorously computed along the trajectory using the dependence of tensor of inertia on the internal vibrational coordinates, and the instantaneous angular momentum vector of O3. In this way, the Coriolis coupling is included and the energy is exchanged between the collisional, rotational and vibrational degrees of freedom, while the total energy is conserved. The total angular momentum is also conserved.

The method is intrinsically parallel: different classical trajectories are propagated on different processors. The vibrational wave packet fits into the memory of one node. We used 128 processors, but easily could employ more, say few thousand.

Our calculations are the most sophisticated calculations of the energy transfer step of ozone presented so far. Our major finding is that the van der Waals states in ozone are very likely to make a significant contribution to the overall formation rate. This is a very interesting new result.

Publications:
1. M. V. Ivanov and D. Babikov, "Mixed Quantum-Classical Theory for the Collisional Energy Transfer and the Rovibrational Energy Flow: Application to Ozone Stabilization", submitted to J. Chem. Phys. (2011).
2. M. V. Ivanov and D. Babikov, "Collisional Stabilization of van der Waals States of Ozone", submitted to J. Chem. Phys. (2011).

Project: Dependence of Secondary Islands in Magnetic Reconnection on Dissipation Model
PI: Paul Cassak, West Virginia University
NERSC Repo: m866
NISE hours awarded: 300,000

My research group was a recipient of NERSC Initiative for Scientific Exploration (NISE) awards in both 2009 and 2010. This summary will have information on both in order to update NERSC on developments since last year's summary was written.

Our 2009 NISE award was entitled "Onset of Collisionless Magnetic Reconnection in Weakly Collisional Plasmas." In last year's report, I summarized the successful completion of the numerical project. At the time, we were about a month away from writing a publication and I said that a graduate student would be presenting the work at conferences later in the year. Since then, we completed our paper and it was submitted, accepted, and published in Physical Review Letters in July of 2010. My graduate student, Luke Shepherd, presented the results at the 2010 Division of Plasma Physics meeting in Chicago in November, 2010, and at the Fall AGU meeting in San Francisco in December, 2010. The paper has been well received, and in less than a year, I am aware of at least 7 publications that have been published recently or will be published soon that have cited the paper.

Our 2010 NISE award was entitled "Dependence of Secondary Islands in Magnetic Reconnection on Dissipation Model." Two projects have been initiated with the additional resources. In the first, a graduate student in my group has performed initial simulations of magnetic reconnection with different dissipation model to investigate the appearance and behavior of secondary islands in these models. Part of the project entailed adding small portions to our code to study different dissipation mechanisms. Simulations and data analysis are ongoing. In a second project, magnetic reconnection with a shear flow on either side of a reconnection site is being studied. Previous work has employed equal and opposite bulk flow velocities on either side, but most applications to naturally occurring reconnection sites require different bulk flow speeds on either side. Simulations with different shear flows on either side have been carried out and are currently being analyzed. Applications for these projects include plasmas in the Earth's magnetosphere, fusion devices, and the solar corona.

Publications

"Comparison of secondary islands in collisional reconnection to Hall reconnection," L. S. Shepherd and P. A. Cassak, Phys. Rev. Lett., 105, 015004 (2010)

Project: Computational Prediction of Protein-Protein Interactions
PI: Harley McAdams, Stanford University School of Medicine
NERSC Repo: m926
NISE hours awarded: 1.9M

We used the NERSC machines for detailed analyses of crystal structures of protein-DNA complexes and for application of the data extracted from the crystals to predict protein binding sites on DNA. This is a classic problem where predictions with

useful accuracy have been elusive. Our computational method involves a completely new, and indeed transformational, way for approaching computational inference of the atomic-level interaction potentials that determine molecular binding kinetics. The atomic-level interaction potentials that we infer from a relatively small set of protein-DNA crystal complexes and the published kinetic information for the respective DNA-protein binding interactions are essentially physical constants relevant to all protein-DNA. We infer these constants entirely from experimental data, which has not been done before.

We have submitted a paper describing our method to Nature. In the paper we show that the atomic-level potentials derived from the training dataset can be used to predict binding sites on DNA of proteins outside the training set with unprecedented accuracy. Indeed, the accuracy of our predictions for more than half of the proteins tested so far is comparable to the accuracy of direct experimental measurements of protein binding motifs. This is a huge result for understanding genetic regulatory pathways in both prokaryotes and eukaryotes. Owing to the large number of potential protein atom-DNA atom interactions at the molecular interface and to combinatorial considerations, we would have been unable to address this problem without the capabilities provided by the NERSC facility.

Project: ITER Rapid Shutdown Simulation
PI: Valerie Izzo, General Atomics
NERSC Repo: m455
NISE hours awarded: 1.2M / 1.0M

The NISE award time was used to simulate a fast shutdown of an ITER plasma with a focus on runaway electron confinement, which must be understood so that ITER discharges can be shut down rapidly without damaging in-vessel components. The ITER simulation was computationally more intensive than similar simulations of existing tokamaks (Alcator C-Mod and DIII-D) both because of its larger size (requiring more grid points) and its longer current quench time (requiring more time steps). A comparison of the ITER simulation with those of the two smaller tokamaks established an apparent strong trend of increasing runaway electron confinement with increasing device size, which has significant implications for runaway electron mitigation strategies in ITER. This result was reported in a talk at the 23rd IAEA Fusion Energy Conference [1] and has been submitted as a paper to Nuclear Fusion.

[1] Izzo, V.A. *et al.,* "Runaway Electron Confinement Modeling for DIII-D, Alcator C-Mod and ITER," 23rd IAEA Fusion Energy Conference, Daejon, Korea, (2010) www-pub.iaea.org/mtcd/meetings/PDFplus/2010/cn180/cn180_papers/ths_9-2.pdf

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Project: Beam Delivery System Optimization of Next Generation X-Ray Light Sources
PI: Ji Qiang, Robert Ryne, Xiaoye Li, Lawrence Berkeley National Laboratory
NERSC Repo: m669
NISE hours awarded: 1.0M

Last year, using the computing time from the NERSC NISE project, we developed and enhanced simulation capabilities that were used in beam delivery system optimization studies for a next generation X-ray light source proposed at Lawrence Berkeley National Laboratory. The results of these studies were included in the CD0 proposal submitted to the DOE, Office of Science. Using this computing time, we also developed and tested a parallel parameter optimization scheme based on a two-level parallelization model. This model uses MPI groups to parallelize the search in parameter space while using the MPI communicator of each group for the calculation of the individual objective function in the parallel simulation. This enables the scalability of the code beyond 10,000 cores. Using this computing time, we also explored a hybrid parallel programming model using a combination of the MPI and OpenMP in the IMPACT code. We implemented OpenMP versions of a number of subroutines in the IMPACT such as the particle pusher with external fields and the parallel 3D FFT. This study is still in process. Some preliminary results will be reported at the SIAM Conference on Computational Science and Engineering in Reno, Nevada.

Project: ILC Damping Ring beam instabilities
PI: Mauro Pivi, Stanford Linear Accelerator Center
NERSC Repo: m669
NISE hours awarded: 260,000

The NISE award program has been extremely useful to give a larger flexibility on the simulation runs used to predict the impact of the electron cloud effect on the Linear Colliders (ILC and CLIC) Damping Rings and has been used to assess the feasibility of a ring with a reduced 3.2 km circumference from the initial 6.4 km. We have used the parallel code C-MAD to predict the beam instability effects in the various ILC damping ring configurations. A reduced damping ring circumference represents a $200M saving for the ILC project that could contribute to make the future machine a reality. Furthermore, to increase the confidence on the simulation codes in use we are closely benchmarking the results with an existing experimental program at Cornell University where the CesrTA 750m long storage ring is dedicated as a test accelerator for the Linear Collider program. Besides, we have started working on the LHC project at CERN Switzerland on the simulation program for the suppression of similar beam instabilities.

Related PUBLICATIONS

1 MATHEMATICAL MODELS OF FEEDBACK SYSTEMS FOR CONTROL OF INTRA-BUNCH INSTABILITIES DRIVEN BY TMCI C. Rivetta et al. In preparation for the PAC11 Conference, New York, April 2011
2 REDUCED MATHEMATICAL MODELS OF TRANSVERSE INTRA-BUNCH DYNAMICS C. H. Rivetta, A. Bullit, J. D. Fox, T. Mastorides, M. Pivi, O. Turgut In preparation for the PAC11 Conference, New York, April 2011
3 EVALUATION OF LIMITS AND PERFORMANCE OF FEEDBACK CONTROL SYSTEM MITIGATING E-CLOUD DRIVEN INSTABILITY IN THE CERN SPS C. Rivetta et al. In preparation for the PAC11 Conference, New York, April 2011
4 ILC DAMPING RING ELECTRON CLOUD R&D EFFORT M. T.F. Pivi et al. In the Proceedings of the ECLOUD10 Workshop, Cornell U., New York, October 2010
5 SINGLE-BUNCH INSTABILITY SIMULATIONS IN CESRTA M. T.F. Pivi and K. Sonnad In the Proceedings of the ECLOUD10 Workshop, Cornell U., New York, October 2010
6 BENCHMARKING OF SIMULATION CODES FOR COLLECTIVE INSTABILITIES K. Sonnad et al. In the Proceedings of the ECLOUD10 Workshop, Cornell U., New York, October 2010
7 TRAPPING OF ELECTRON CLOUD IN ILC/CESRTA QUADRUPOLE AND SEXTUPOLE MAGNETS L. Wang and M. T.F. Pivi In the Proceedings of the ECLOUD10 Workshop, Cornell U., New York, October 2010
8 ELECTRON CLOUD MITIGATION INVESTIGATIONS AT CESR-TA J. Calvi et al. In the Proceedings of the ECLOUD10 Workshop, Cornell U., New York, October 2010
9 RECOMMENDATION FOR THE FEASIBILITY OF MORE COMPACT LC DAMPING RINGS M. T.F. Pivi et al. In the Proceedings of the IPAC10 Conference, Kyoto, Japan, May 2010
10 COLLECTIVE EFFECTS IN THE SUPERB COLLIDER T. Demma and M. Pivi In the Proceedings of the IPAC10 Conference, Kyoto, Japan, May 2010
11 THE SUPERB PROJECT ACCELERATOR STATUS M. E. Biagini et al. In the Proceedings of the IPAC10 Conference, Kyoto, Japan, May 2010
12 INDUCED CYCLOTRON RESONANCES OF THE ELECTRON CLOUD IN DIPOLE MAGNETS S. De Santis et al. In the Proceedings of the IPAC10 Conference, Kyoto, Japan, May 2010
13 APPLICATION OF AN ELECTRON CLEARING ELECTRODE TO A BEAM PIPE FOR WIGGLER MAGNETS IN KEKB POSITRON RING Y. Suetsugu, H. Fukuma, K. Shibabta, M. Pivi and L. Wang In the Proceedings of the IPAC10 Conference, Kyoto, Japan, May 2010
14 CESRTA RETARDING FIELD ANALYZER MEASUREMENTS IN DRIFTS, DIPOLES AND WIGGLERS J. Calvi et al. In the Proceedings of the IPAC10 Conference, Kyoto, Japan, May 2010
15 LONG LIFETIME ELECTRON CLOUD IN WIGGLER AND QUADRUPOLE MAGNETS OF CESRTA L. Wang and M. Pivi In the Proceedings of the IPAC10 Conference, Kyoto, Japan, May 2010
16 PROGRESS IN STUDIES OF ELECTRON-CLOUD INDUCED OPTICS DISTORSION AT CESRTA J. Calvi, J. A. Crittenden et al. In the Proceedings of the IPAC10 Conference, Kyoto, Japan, May 2010
17 ELECTRON CLOUD AT LOW EMITTANCE IN CESRTA Mark A. Palmer et al. In the Proceedings of the IPAC10 Conference, Kyoto, Japan, May 2010

Project: First Principles Modeling of Charged-Defect-Assisted Loss Mechanisms in Nitride Light Emitters
PI: Emmanouil Kioupakis, University of California, Santa Barbara
NERSC Repo: m934
NISE hours awarded: 900,000

We made use of our NISE award to investigate charged-defect-assisted loss processes in nitride light emitters. Charged defects may be present in every material and can scatter charge carriers in an optoelectronic device. This scattering enables indirect nonradiative recombination or absorption processes that are detrimental to the device performance. We

used a screened Coulomb potential to model the scattering by the defects and investigated the magnitude of charge-defect-assisted Auger recombination and free-carrier absorption in nitride materials. We found that charge-defect-scattering is not the major mechanism that contributes to the efficiency degradation for realistic defect concentrations. On the other hand, we identified electron-phonon coupling and alloy scattering as the main scattering processes that assist the loss mechanisms. Based on our findings, we proposed ways to mitigate the effect of the loss and improve the performance of nitride light emitters.

Publications:

E. Kioupakis, P. Rinke, K. T. Delaney, and C. G. Van de Walle, Indirect Auger recombination as a cause of efficiency droop in nitride LEDs, submitted.

E. Kioupakis, P. Rinke, and C. G. Van de Walle, Determination of internal loss in nitride lasers from first principles, *Appl. Phys. Express* **3** (2010) 082101

E. Kioupakis, P. Rinke, A. Schleiffe, F. Bechstedt, and C. G. Van de Walle, Free-carrier absorption in nitrides from first principles, *Phys. Rev. B* **81** (2010) 241201(R)

Project: High Resolution Climate Simulations with CCSM
PI: Warren Washington, NCAR
NERSC Repo: mp9
NISE hours awarded: 3.5 M

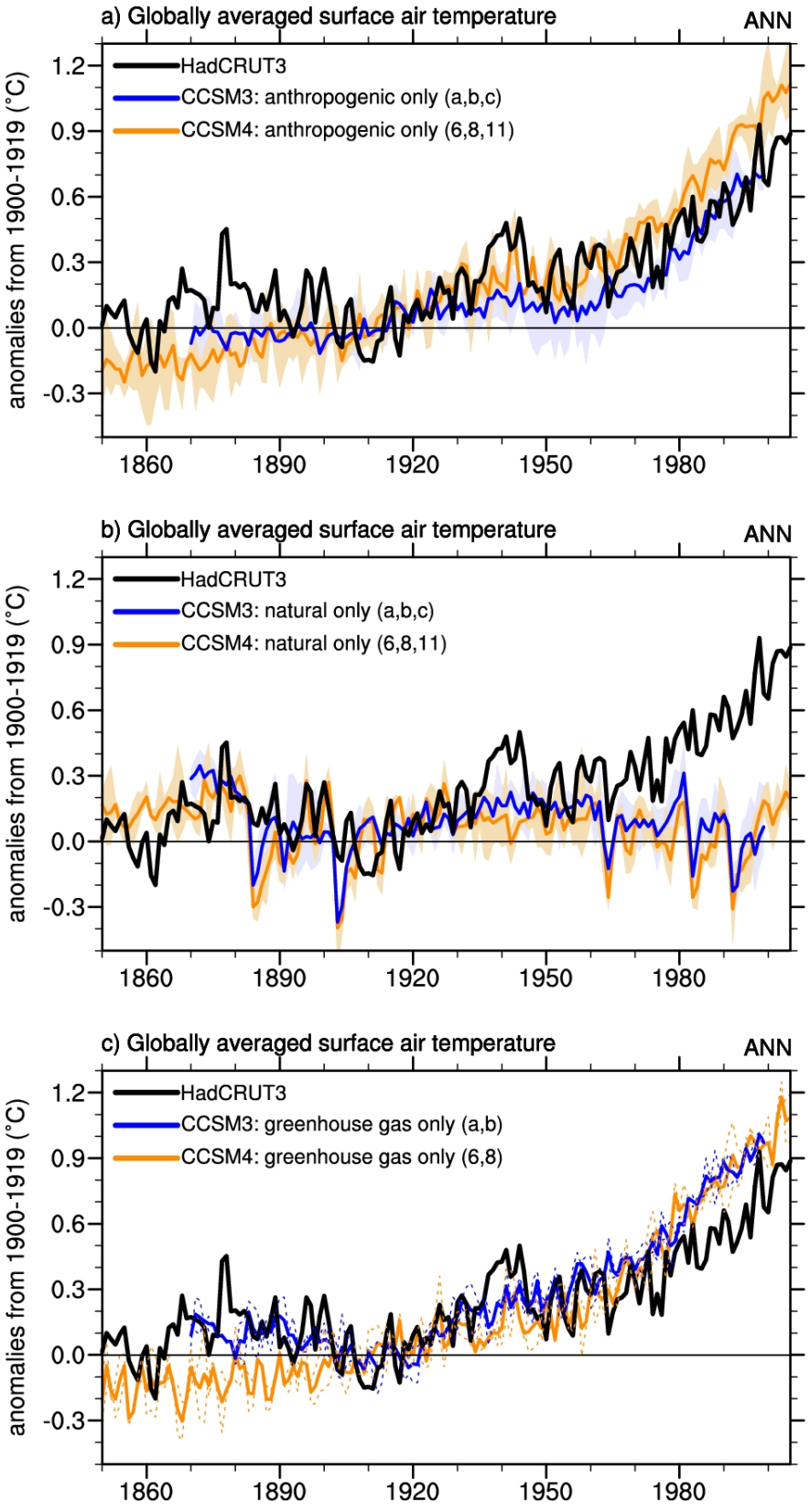
The high resolution version of CCSM – with a 0.5 degree atmospheric model coupled to a 1.0 degree ocean model as well as state-of-the-art sea ice and land surface scheme– had previously encountered a numerically unstable polar night jet near the poles. The instability has been treated, and the need exists to tune the model to a zero radiative balance to allow climate change simulations. Our intention was to bring the model into radiative balance with a 40-year simulation, then produce a control simulation followed by a 20^{th} century simulation to provide a baseline comparison for future decadal prediction experiments.

The 40-year simulation was delayed due to the opportunity to upgrade to the Community Atmospheric Model (CAM). With the permission of NERSC management, we diverted the remaining NISE allocation to experiments in preparation of the IPCC AR5. Single forcing experiments for the 20th Century have been underway with the CCSM4. Our goal is to complete a modest sized ensemble for each forcing scenario. In these experiments the CCSM4 is forced separately with each external forcing, i.e., volcanic, solar, greenhouse gases, black carbon & sulfate aerosols, land use and ozone, in order to isolate the mechanisms by which each impacts the climate. We have also completed three ensemble members of anthropogenic-and natural-only with another two currently running. Initial analysis of these single forcing runs is included in Meehl et al. (2011).

For example, the following figure shows the global temperature time series from the observations (black) and CCSM3 and CCSM4 anthropogenic-only, natural-only and greenhouse-gas-only experiments. The natural forcings do a good job in CCSM4 of producing the early part of the observed temperature record from 1850 to about 1935, anthropogenic-only experiments perform best compared to observations from the late-1930s onward, and GHG-only are too cool early, and too warm later on with a more gradual warming trend throughout.

Publications

Meehl G.A., W.M. Washington, J.M. Arblaster, A. Hu, H. Teng, C. Tebaldi, J.B. White III and W.G. Strand, 2011: Climate system response to external forcings and climate change projections in CCSM4, *J Climate*, in preparation.


a) Globally averaged surface air temperature
ANN
HadCRUT3
CCSM3: anthropogenic only (a,b,c)
CCSM4: anthropogenic only (6,8,11)
anomalies from 1900-1919 (°C)
1.2
0.9
0.6
0.3
0.0
-0.3
1860
1890
1920
1950
1980
b) Globally averaged surface air temperature
ANN
HadCRUT3
CCSM3: natural only (a,b,c)
CCSM4: natural only (6,8,11)
anomalies from 1900-1919 (°C)
1.2
0.9
0.6
0.3
0.0
-0.3
1860
1890
1920
1950
1980
c) Globally averaged surface air temperature
ANN
HadCRUT3
CCSM3: greenhouse gas only (a,b)
CCSM4: greenhouse gas only (6,8)
anomalies from 1900-1919 (°C)
1.2
0.9
0.6
0.3
0.0
-0.3
1860
1890
1920
1950
1980

Project: In-house Transport Simulator based on Non Equilibrium Green's Function
PI: Sayeef Salahuddin, EECS, UC Berkeley
NERSC Repo: m946
NISE hours awarded: 0.6 M

Our main focus with the hours awarded by NISE-2010 was to massively parallelize our in house code for solving quantum transport problems. As the core device model, we use Non Equilibrium Green's Function (NEGF) formalism that is a fundamental statistical quantum mechanical approach for non-equilibrium problems. The theory is well documented and established. The fundamental equations to solve are:

$$(E-H-\Sigma^{R}-\Sigma^{S})G^{R}=I \text{ and } (E-H-\Sigma^{R}-\Sigma^{S})G^{<}=\Sigma^{<}G^{A} \quad (1)$$

The mathematical and numerical objects are total energy E, the electronic device Hamiltonian H, self-energies Σ^{R},Σ^{S}, $\Sigma^{<}$, the electron propagators G^{R} and G^{A} and the electron correlation function $G^{<}$. H is the Hermitian Hamiltonian matrix of size (atoms) x basis (can be as high as 300) that is sparse in a local orthogonal basis. Σ^{R} is a full non-Hermitian matrix of size (atoms at the open contact x basis size). Σ^{S} is also called the so-called scattering self-energy that regulates the out-scattering into other channels due to incoherent interactions. $\Sigma^{<}$ is the injection self energy due to contacts and scattering. The computational complexity can be briefly summarized as follows:

The numerical problem is different from typical linear solution problems where a column of AX=B is sought after, but all diagonal blocks of G^{R} and all diagonal and super diagonal blocks of $G^{<}$ are needed. With the matrices being of the size of 10^{6}-10^{8}, this becomes almost an intractable problem without efficient algorithms that take advantage of the physical symmetry of the problem.

Using the hours awarded, we have achieved great success in solving this problem. Fig. 1 shows scaling behavior of our transport code. Perfect scaling up to 8,192 cores has been achieved. This massive parallelization has enabled us to solve problems that have been deemed intractable before. This resulted in multiple publications in leading journals including *an issue cover story [1-5]*.

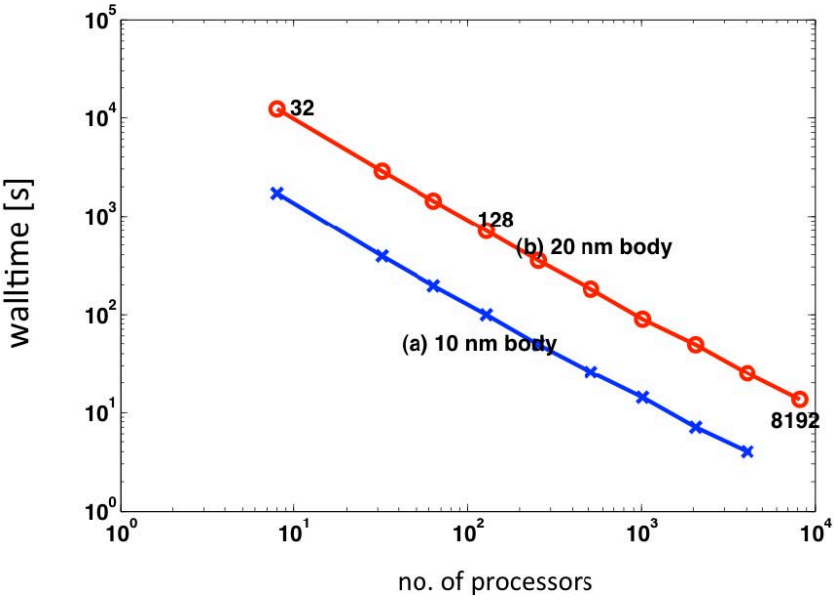


Fig. 1. Scaling behavior for a 2D InAs channel with (a)10 nm and (b) 20 nm body thickness for one single bias point on Franklin. 1000 Energy points and 15 transverse k points are considered. For this study 2 levels of parallelization were incorporated. The profiling was done using IPM (Integrated Performance Monitoring) available on Franklin.
(http://www.nersc.gov/nusers/resources/software/tools/ipm.php)

Publications:

Salahuddin, S., "Barrier-free tunneling in a carbon heterojunction transistor," *Appl. Phys. Lett.*, 2010. *[issue cove story]*
Yoon, Y. and S. Salahuddin, "Analysis of InAs vertical and lateral band-to-band tunneling transistors: Leveraging vertical tunneling for improved performance," *Appl. Phys. Lett*., 2010.
Salahuddin, S., "Inverse temperature dependence of subthreshold slope in graphene nanoribbon tunneling transistors," *Appl. Phys. Lett*., 2010.
Kim, S. and S. Salahuddin, "Performance analysis of carbon-based tunnel field-effect transistors for high frequency and ultralow power applications," *Appl. Phys. Lett*., 2010.
Ford, A., et al., "Ultrathin compound semiconductor on insulator layers for high-performance nanoscale transistors," *Nature*, 2010.