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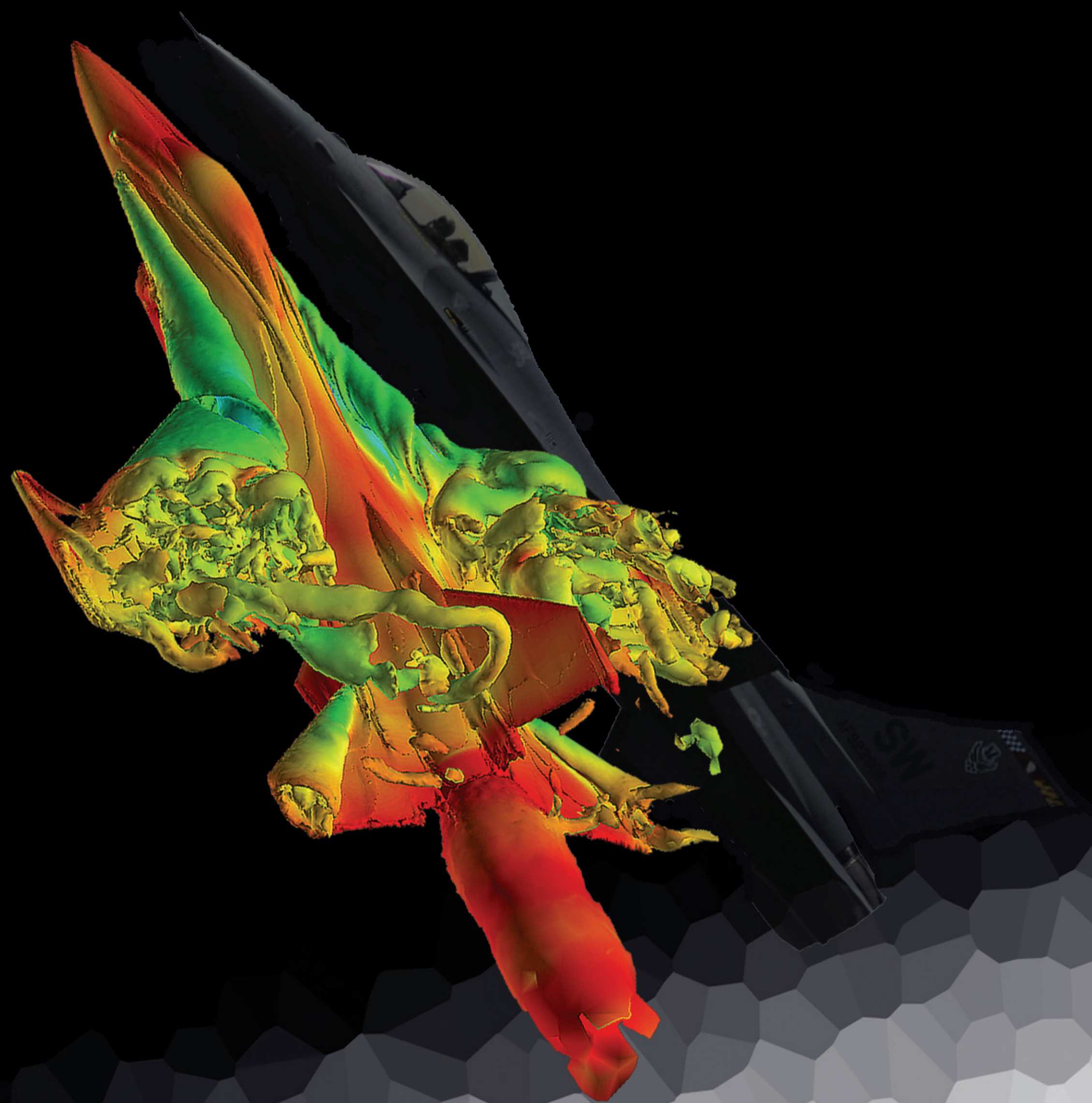

Application Briefs 2008

A Center of the Air Force Research Laboratory
Managed by the University of Hawaii

MAUI HIGH PERFORMANCE COMPUTING CENTER

APPLICATION BRIEFS 2008

Air Force Maui Optical & Supercomputing Site (AMOS)

MAUI HIGH PERFORMANCE COMPUTING CENTER

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WELCOME

This is the fourteenth annual edition of Maui High Performance Computing Center's (MHPCC) *Application Briefs* which highlights some of the successes our staff and customers have achieved this year.

MHPCC, established in September 1993, is an Air Force Research Laboratory (AFRL) Center managed by the University of Hawaii. A leader in scalable parallel computing technologies, MHPCC is chartered primarily to support the Department of Defense (DoD) and other federal government organizations.

MHPCC offers an innovative environment for High Performance Computing (HPC) applications. This includes:

- Computational Resources: Stable and secure parallel computing platforms for prototyping, benchmarking, and testing applications. MHPCC is ranked as one of the top HPC centers in the Department of Defense in terms of computational capabilities.

- High-Speed Communications Infrastructure: OC12 connections, offering 620 megabit per second (Mbps) capacity, provide direct access to MHPCC resources — over the Defense Research and Engineering Network (DREN) and the Hawaii Intranet Consortium (HIC).

- Support Services: An expert staff provides MHPCC users with systems, network, and applications support in addition to assistance with code porting, optimization, and application development.

MHPCC is a well-established member of the High Performance Computing community, participating in collaborations and partnerships that extend its capabilities. MHPCC is a direct contributor to the Department of Defense as a (an):

- Allocated Distributed Center within the DoD High Performance Computing Modernization Program (HPCMP). MHPCC provides resources to the DoD research community, as well as Pacific Region DoD organizations, including the Air Force's Maui Space Surveillance Complex.

- Center within the Air Force Research Laboratory. MHPCC works closely with DoD and other government researchers to support Research, Development, Testing, and Evaluation (RDT&E) efforts.

- Air Force Research Laboratory resource for the Air Force Maui Optical & Supercomputing Site (AMOS).

- Member of Hawaii's growing science and technology community.

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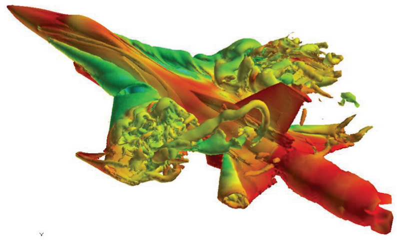
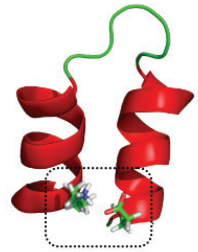
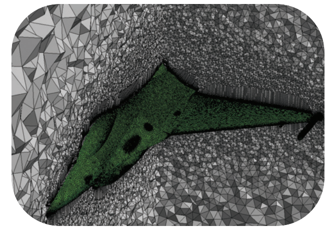
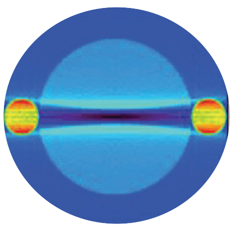
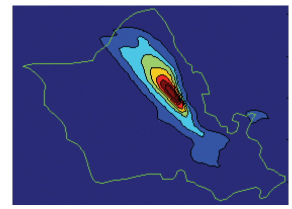
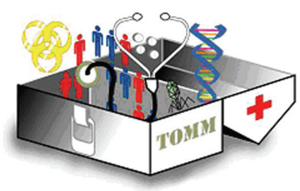
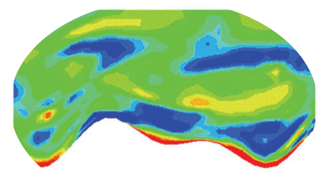




APPLICATION BRIEFS

The user application briefs in this publication represent selected research efforts that have taken place at MHPCC during 2008. Each Application Brief was written by an individual researcher or research team, and reflects their first-hand experiences using MHPCC resources. These articles reflect the diverse nature of our users and projects.



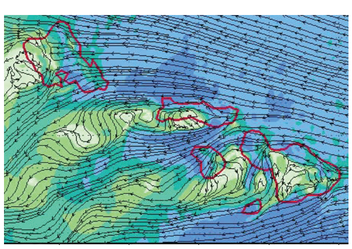
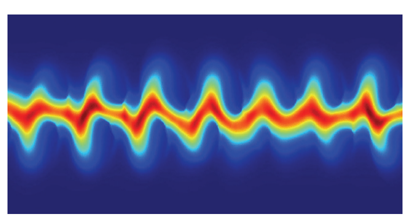
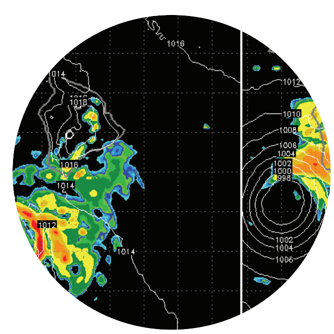


The Application Briefs in this document are the result of the efforts of more than 30 authors. We acknowledge the contributions of each of these individuals and are grateful for their work. We welcome back those authors who have become regular and frequent contributors. We also welcome those making their MHPCC Application Briefs debut this year.

The shaded box at the top of each brief's first page is a short summary of the article. Author and/or organizational contact information can be found in the shaded box at the end of each brief. The notation at the bottom of each page indicates each project's primary functional area (DoD, Government, or Academic).


All the efforts described in this document were performed using resources provided by the Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP). Additional sponsorship has come from a variety of Research, Development, Test and Evaluation sources, including the Offices of Research and the Research Laboratories in the Defense Services.

Thank you for your support.

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Computational Stability and Control Analysis of the F-16

Keith Bergeron, Scott A. Morton, Dave McDaniel, John Dean

This computational research project is advancing the techniques needed to conduct virtual flight-testing through the simulation of an F-16 performing flight maneuvers, including the effects associated with control surface movements and response to aerodynamic loads.

Project Overview: Historically, aerodynamic stability and control engineers have used an iterative process combining semi-empirical lower-order, wind-tunnel, and flight test modeling techniques to determine the aerodynamic characteristics of new fighter aircraft. Unfortunately despite their best efforts using the best available predictive capabilities, nearly every major fighter program since 1960 has had costly nonlinear aerodynamic or fluid-structure interaction issues that were not discovered until flight testing.[1] Using advanced computational fluid dynamics (CFD) methods, simulations are now capable of capturing the unsteady nonlinear aerodynamic behavior that leads to the various static and dynamic instabilities associated with highly-maneuverable aircraft. More precisely, the computational tools include advanced meshing techniques, hybrid turbulence modeling, and systems identification analyses. This cutting-edge computational approach could potentially save billions of dollars in aircraft design, acquisition, and certification.

Reference:

1) McDaniel, D.R., Cummings, R.M., Bergeron, K., Morton, S.A., and Dean, J.P., "Comparisons of CFD Solutions of Static and Maneuvering Fighter Aircraft with Flight Test Data," 3rd International Symposium on Integrating CFD and Experiments in Aerodynamics, June 2007.

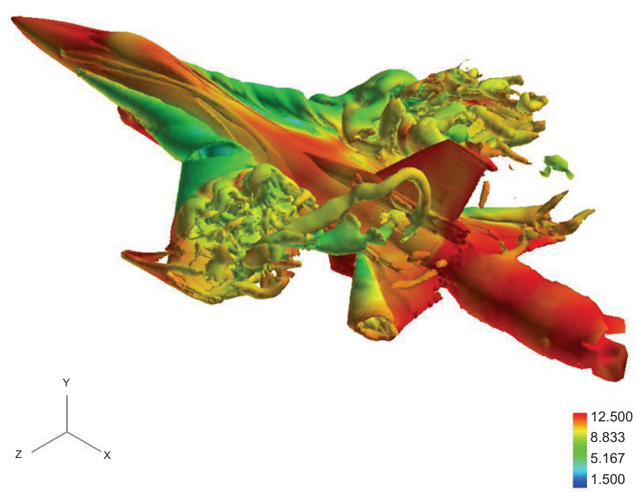

Figure 1. CFD simulation of the F16 – C , at Mach = 0.6, 5,000 ft., 25 deg. AOA, Vorticity Iso-surface (1,000/sec.), and colored by pressure (psi).

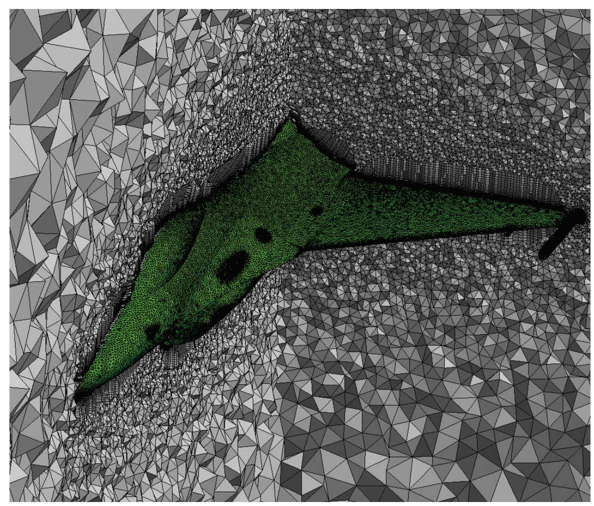

Figure 2. F-16 Grid for high-fidelity simulations.

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Resources: 256-1,024 processors on *Jaws* at MHPCC, 512 processors on *Hawk* and *Falcon* at AFRL, 128-256 processors on *Iceberg* and *Midnight* at ARSC, 256 processors on *Babbage* at NAVO, and 128 processors on *Blackbird* at USAF Academy
Sponsorship: DoD HPC/AF SEEK Eagle Office Institute for High Performance Computing Applications of Air Armament (IHAAA), DoD High Performance Computing Modernization Office (HPCMP), Arctic Region Supercomputing Center (ARSC), Air Force Office of Scientific Research (AFOSR), and the National Research Council (NRC)
Acknowledgement: USAF Academy Modeling and Simulation Research Center

Maritime Domain Awareness (MDA) Prototype Acceleration Project Support

Robert Dant and Glenda Ramos

The MDA Prototype System attempts to collect, analyze, assess, and disseminate intelligence in defending the United States from maritime threats. This is an initiative of the United States Coast Guard (USCG) and Department of Homeland Security (DHS) to create a national command, control, communications, computers, intelligence, surveillance, and reconnaissance (C4ISR) capability, monitoring all ports, coasts, and navigable waterways within the United States. A Service-Oriented Architecture (SOA)-based environment was established for the MDA prototype.

Objective: The objective of this project was to provide MHPCC resources to support Maritime Domain Awareness (MDA) Prototype Acceleration (Spiral 2) activities that focused on extending and enhancing the MDA capabilities fielded during Spiral 1. MDA technologies of interest were: (1) Vessel Tracking, (2) Cargo Monitoring, (3) People Screening and Identity Management, (4) Maritime Interdiction Operations, (5) Broad-based Collaboration, and (6) Information Management, Database, Service-Oriented Architecture, and Interoperability.

Figure 1. A major part of the MDA Spiral 1 was vessel tracking.

Figure 2. MDA will create a national C4ISR capability to monitor all major U.S. ports.

Methodology: In order to accelerate the development of an enhanced MDA prototype, our research efforts were focused on Developing a Data Warehouse capability by:

- Demonstrating the Vessel and Cargo Tracking capabilities using a Service-Oriented-Architecture (SOA)-based environment
- Developing capabilities to select relevant records in the database that could quickly match "people of interest"
- Developing the capability to generate queries to retrieve maritime cargo details
- Demonstrating the capability to identify suspicious activities at Port X during Timeframe Y
- Processing "Involved Parties" for selected ships and containers (e.g., ship owner, shipper, consignee, etc.)
- Developing a "proof of concept" demonstration

Results: MHPCC developed an MDA proposal in response to a SPAWAR PEO C41 BAA and supported MDA activities with Boeing Phantom Works (Huntsville, AL and Huntington Beach, CA). The management and staff at MHPCC participated in the PACOM Tech Expo held at Pearl Harbor and supported the "Intelligence Fusion" Demo. The demo was conducted during a PACOM (Pacific Command) Tech Expo at Pearl Harbor Naval Base, 13-14 Feb 08.

A Service-Oriented Architecture (SOA)-based environment was developed for the prototype. The Oracle SOA Suite was chosen to support the SOA-based infrastructure. Within the Oracle SOA Suite, the JDeveloper component was used to develop the Web Services that support the technologies of interest such as the Vessel Tracking and Cargo Monitoring. With the SOA-based implementation of these web services, these web services are made to easily interoperate with any existing systems within MDA.

Figure 3. A key element of MDA Spiral 1 was cargo monitoring.

Significance: The MDA Prototype System attempts to collect, analyze, assess, and disseminate intelligence in defending the United States from maritime threats. This is an initiative of the United States Coast Guard (USCG) and Department of Homeland Security (DHS) to create a national command, control, communications, computers, intelligence, surveillance, and reconnaissance (C4ISR) capability, monitoring all ports, coasts, and navigable waterways within the United States.

By accelerating an MDA Prototype System through the use of MHPCC resources, the decision-makers now have a better look at how data from disparate sources can best be integrated. Using a Service-Oriented Architecture (SOA)-based approach, cargo and ship information (and other related databases) can be delivered to the right people at the right time. Web Services can now be viewed at an early stage, and can be reusable by multiple applications across different intelligence platforms.

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Resources: Various Software Development Servers at MHPCC
Sponsorship: Office of Naval Research (ONR)

Effect of Hawaii's Big Island on Hurricanes

Christopher Chambers and Tim Li

Numerical simulation results suggest that the Big Island plays an important role in protecting the smaller heavily populated Hawaiian Islands to its west by weakening the strength of hurricanes approaching from the east. Five previous Hawaiian hurricanes are numerically simulated.

Project Overview: Numerical simulations with the Weather Research and Forecasting model are conducted to investigate how the Big Island of Hawaii might impact the track and intensity of approaching hurricanes. Hurricanes Dot (1959), Iniki (1992), Daniel (2000), Jimena (2003), and Flossie (2007) are simulated. Each case is run twice, one with the presence of orography of the Big Island and the other with the island replaced with open ocean.

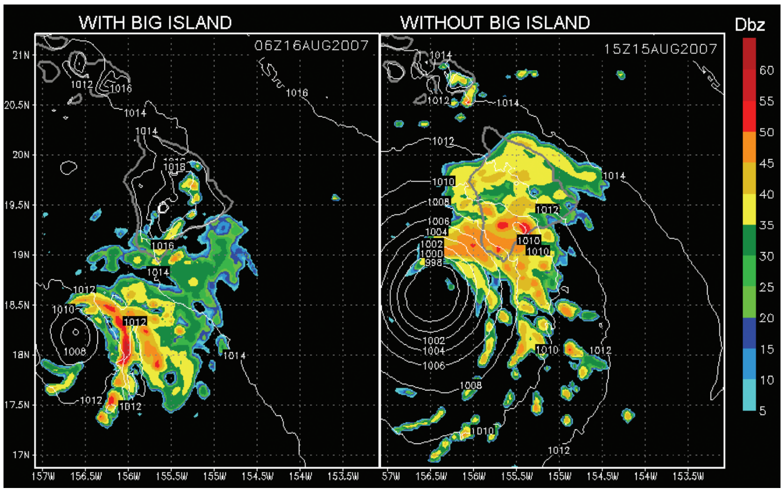

Figure 1 shows the simulations of Hurricane Flossie. The presence of the Big Island orography leads to a weakening of the storm intensity and a southward deviating track. Figure 2 shows a landfalling example based on Hurricane Dot. While the track of the hurricane does not change much, its intensity experiences a significant difference. A well organized rainband structure with much lower minimum sea level pressure appears in the case when the Big Island is removed.

Figure 1. Sea level pressure (unit: mb) and composite radar reflectivity (unit: Dbz) for the Hurricane Flossie (2007) simulations with (left panel) and without (right panel) the Big Island. The different times indicate that the Big Island slows the storm such that it takes 15 extra hours to reach 156.5W.

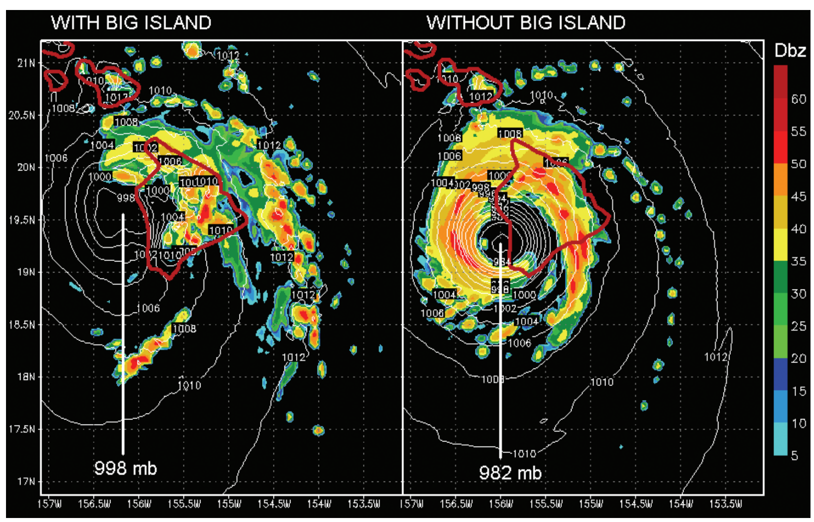

Figure 2. As Figure 1 but for a Hurricane Dot (1959) simulation with the initial storm displaced north 135 km to produce a Big Island landfall.

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Resources: IBM P4: *Hurricane* Cluster at MHPCC and Department of Meteorology, University of Hawaii: Sun workstations
Acknowledgement: University of Hawaii's Department of Meteorology at Manoa

High Fidelity CT Imaging of High-Z Materials for Rocket Motor Aging Detection

Robert Levine, Xuemin Jin, Gregory Ruderman, Don Wickham

Propellant aging in solid rocket motors can result in defects such as micro-cracks, fissuring, and abnormal density variations. These defects can lead to abnormal burn rates and unsafe operations of the motor. High energy γ-ray CT is a nondestructive inspection method to evaluate structural integrity of a rocket motor. Various artifacts in the reconstructed image due to high-Z beam hardening and scattering can hinder the detection of defects and subtle changes due to aging. In this project high fidelity Monte Carlo simulation of γ-ray interaction and transport through solid rocket motors is employed to characterize such artifacts. New beam hardening and scatter mitigation algorithms based on the MHPCC simulation are being developed and applied to projected CT data. Sufficient statistics with rocket dimensions require parallel Monte Carlo simulation with > 1,000 processors for 10-20 billion input particles. Beam hardening and scattering corrections will be verified with real data CT reconstructions.

Research Overview: Evaluating the integrity of large solid rocket motors is critical for the maintenance of a safe, reliable and effective ICBM force. As the polymer substrate in the propellant ages, slow chemical and physical processes can result in micro-cracks, fissuring, separation from the liner, and abnormal polymer density variation. A degraded propellant may result in asymmetric and abnormal burn rates for an unsafe and unreliable rocket. Computer Tomography (CT) provides a practical nondestructive testing (NDT) method to verify the integrity and monitor aging of large rocket motors. The technique is analogous to medical imaging CT, but with much higher energies for increased penetration and reduced scattering. Nevertheless, the presence of high-Z materials (typically metal components) in rocket motors leads to significant artifacts that hinder the detection of defects and subtle aging effects in the solid rocket propellant.

The complexity of high-energy particle interactions in rocket motor materials necessitates the application of forefront simulation codes to predict transmitted fluence into the detector. This is particularly true in heterogeneous materials with sharp high-Z boundaries, and especially if high-Z artifacts from multiple views are being combined into a reconstructed image. Recent technological advances in computing power have made it possible to carry out high energy physics simulations to a precision previously unimaginable. In this research, we are taking advantage of this advance to develop tools for the complete physics characterization of rocket motor NDT. We use high fidelity Monte Carlo simulation of γ-ray interaction and transport through solid rocket motors to characterize and mitigate CT artifacts and noise due to high-Z materials. The applications of this approach extend beyond the specific problems of CT artifacts to a basic understanding of the interactions and measurements in high-energy imaging.

For rocket motor inspection, two distinct conditions drive our research in CT imaging: 1) the detection of extremely small (<5 mm) and low contrast aging effects, and 2) the observation of these effects among high-Z components in the motor. It is well-known that two physics-based effects, beam hardening and scattering, create distinctive artifacts with spatial frequencies in the reconstruction that are much greater than in the measured profile.[1] This fact has its origin in the view dependence of the effects against the primary fluence, a dependence that enters into the overall reconstruction by back projection. Because of high attenuation, the high-Z components in the rocket motor cause both masking effects and view dependence. Beam hardening artifacts arise from the incident polychromatic γ-ray source and the fact that the linear attenuation coefficient usually decreases with energy. As such, the low energy photons are absorbed preferentially and the detected photons become proportionally higher energy. This effect can be significant. For example, beam hardening can cause a "whitening" effect near the edges of an image as shown in Figure 1. Another artifact is the appearance of streaks and flares in the vicinity of larger density components and between those components. A γ-ray beam traveling through an object is attenuated by absorption or scattering. Scattering attenuation occurs because some of the original photons in the beam are deflected. For example, as measured by energy loss, 1 MVp γ-rays in steel have ~50% attenuation by scattering and ~50% by absorption (mostly into Compton electrons). Unlike with beam hardening, air affects the measured scatter by providing larger dispersal distances along the primary fluence trajectory. The directional dependence of scatter can cause prominent streaks in the reconstructed image as depicted in Figure 1.

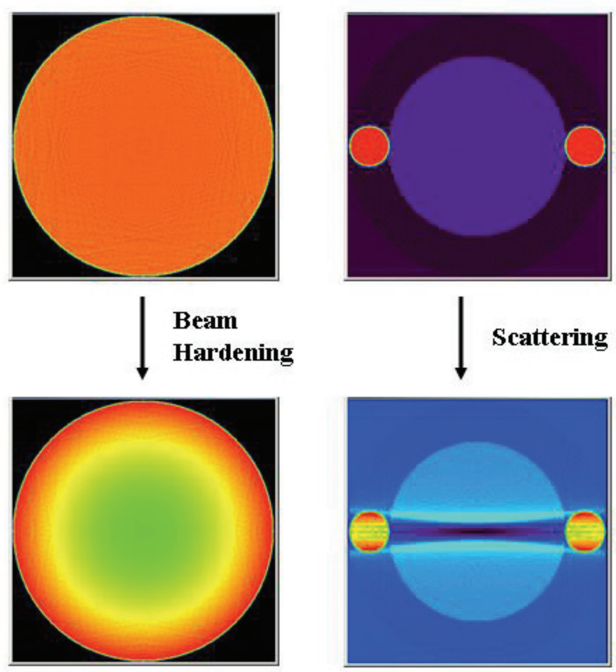

Figure 1. Artifacts arising from beam hardening (left) and scattering (right).

We are currently developing artifact mitigation algorithms based on Monte Carlo simulation using the MHPCC *Jaws* system. The BEAM/DOSXYZ Monte Carlo code is based on the SLAC EGS4 codes that were developed to simulate detector response from high-energy accelerator beams.[2] Taking as input the γ-ray and charge particle cross sections and stopping powers, the system predicts the interactions, transport, and energy deposition for particles with energies in the range of 10 keV - 50 MeV. Gamma ray interaction and transport is modeled with individual Rayleigh, photoelectric, Compton, and pair production interaction cross sections. The cross sections stochastically define the γ-ray transport range and interaction type. For electron transport, high-energy secondary rays resulting from knock-on electrons and hard bremsstrahlung are separated from continuous energy deposition due to multiple scattering. User-defined energy thresholds specify the creation and transport of secondary rays as independent particles for both photons and electrons. In addition to EGS4-based particle transport, BEAM/DOSXYZ allows user-defined specification of accelerator, target, and film dose phantoms.

Figure 2 shows a simulation phantom scaled to the specifications of the Hill AFB NDT accelerator, detector and physical dose phantoms. The tungsten target, collimators, and four meter diameter water phantom with a 10 cm cylindrical steel core are shown in the figure. The detector slab is sodium iodide scintillator. In this simulation a scoring plane was defined in the beam line just ahead of the scintillator in order to characterize the fluence incident on the detector. The BEAM/DOSXYZ system allows for the specification of latch bits for each particle in the scoring plane phase space. Because the latch bits contain information about the particle trajectory and interactions, primary γ-rays can be distinguished from scatter. Figure 3 shows the primary photon fluence, all particle scatter, and charged particle scatter into the detector resulting from a BEAM/DOSXYZ simulation with 12.8 billion input particles computed on 1,280 processors of the MHPCC *Jaws* system. The simulation required less than four hours. Figure 4 contains the energy spectrum from the same populations of scoring plane particles. The results demonstrate the excellent statistics achievable on the MHPCC system even for high energy particle transport through meters of material. We are continuing a series of calculations necessary to generate inputs to CT artifact mitigation algorithms for rocket motor NDT.

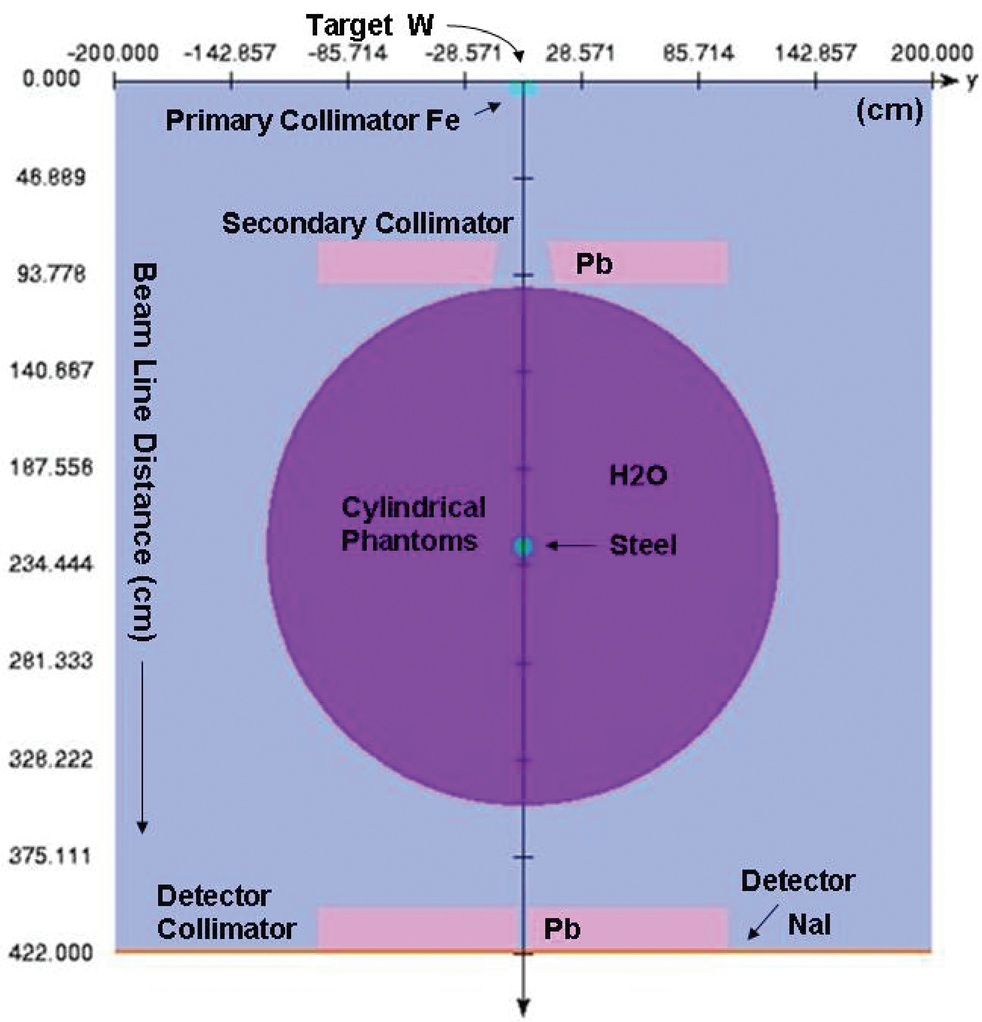

Figure 2. Dose phantom for Monte Carlo simulation of high energy particle transport through a rocket motor. Component identification, materials, and scoring plane are indicated in the figure.

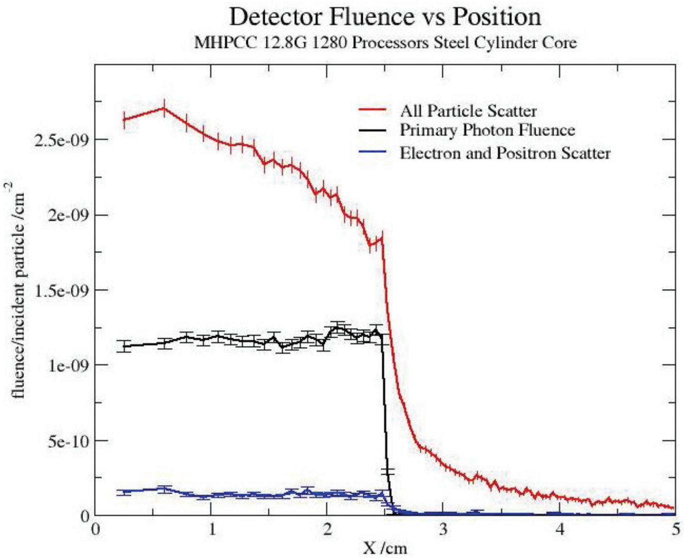

Figure 3. Scoring plane fluence versus position resulting from 12.8 billion input electrons to the BEAM/DOSXYZ code with the phantom in Figure 2. Simulation run on 1,280 MHPCC processors. Latch bit determined particle fluence for primary photons, all particle scatter, and charge particle scatter shown.

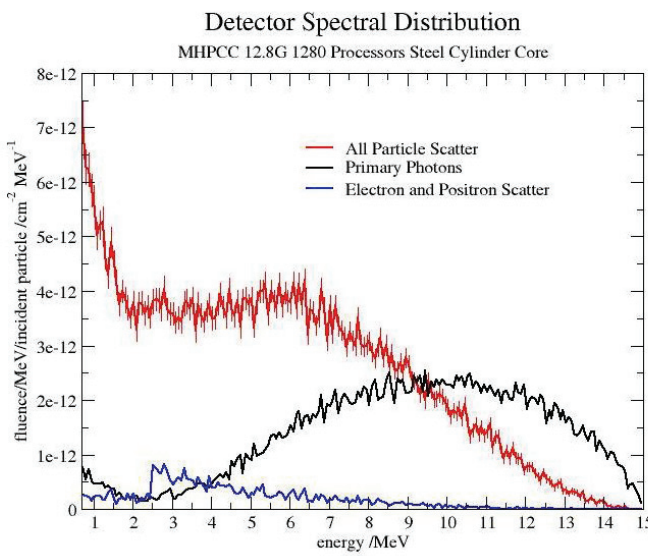

Figure 4. Scoring plane energy spectrum resulting from 12.8 billion input electrons to the BEAM/DOSXYZ code with the phantom in Figure 2. Simulation run on 1,280 MHPCC processors. Latch bit determined spectra for primary photons, all particle scatter, and charge particle scatter shown.

References:

1) Glover, G.H., "Compton scatter effects in CT reconstructions," *Med. Phys.*, 9, 860-867, Nov./Dec. (1982).
2) Rogers, D.W.O., Faddegon, B.A., Ding, G.X., Ma, C.-M., We, J. and Mackie, T.R., "BEAM: A Monte Carlo code to simulate radiotherapy treatment units," *Med. Phys.,* 22, 503-524, (1995).

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Resources: *Jaws* at MHPCC (Dell PowerEdge 1955 systems)
Sponsorship: DoD AFRL

Orographic Influences on Oahu Floods

Michael Murphy and Steven Businger

Thunderstorms form and become anchored along the Ko'olau Mountain range, often resulting in flash floods. To investigate the impact of terrain in this case, the event was simulated using the Weather Research Forecasting (WRF-ARW) numerical model with a very high grid resolution (500 m) over Oahu.

Research Summary: Heavy rainfall events and flashfloods represent a significant weather hazard in the Hawaiian Islands that has proven challenging for forecasters. Under conditions of easterly low-level flow and unstable atmosphere, thunderstorms form and become anchored along the Ko'olau Mountain range, often resulting in flash floods. A typical event occurred on 2 April 2006 when deep convection resulted in more than eight inches of rainfall on saturated windward slopes producing a flash flood. To investigate the impact of terrain in this case, the event was simulated using the Weather Research Forecasting (WRF-ARW) numerical model with a very high grid resolution (500 m) over Oahu. The model reproduced the impact of the terrain on the flow (Figure 1), resulting in convective storms over the Ko'olau range in a pattern and location similar to observations (Figure 2). The results suggest that in the future very high-resolution simulations may be able to provide accurate flood forecast guidance in the case of anchored thunderstorms.

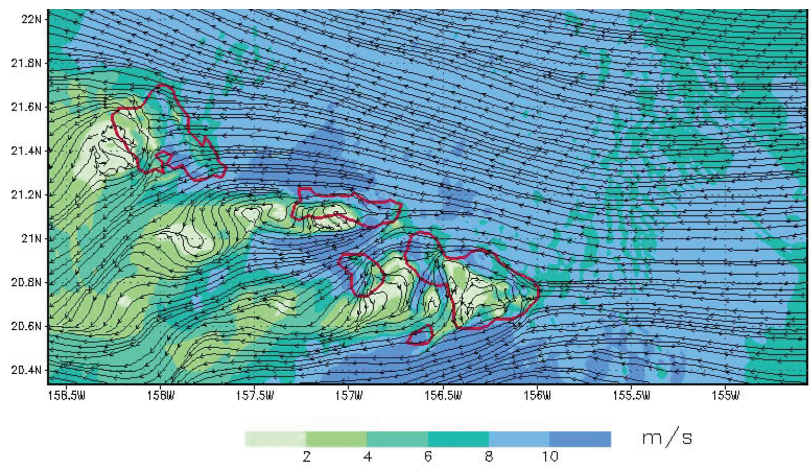

Figure 1. Predicted surface streamlines and wind speed (m s^{-1}) at 1000 HST.

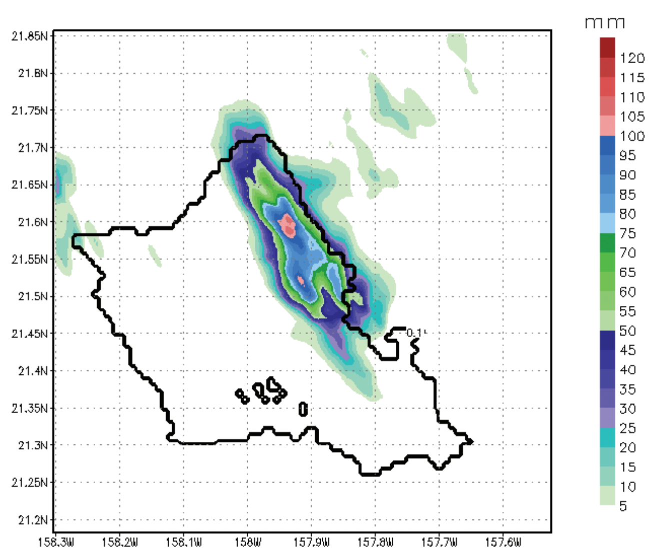

Figure 2. Predicted total rainfall (mm) for the storm period (0700 - 1400 HST).

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Resources: IBM P4 *Hurricane* cluster at MHPCC
Sponsorship: NOAA

Higher-Order Algorithms for Advanced Plasma Models

Uri Shumlak, Bhuvana Srinivasan, Robert Lilly

This project uses the WARPX (Washington Approximate Riemann Plasma) code developed at the University of Washington. The high-resolution wave propagation method (a finite volume method) and the Runge-Kutta, discontinuous Galerkin method (a finite element method) are employed for their ability to capture solutions with high speed flows and sharp gradients.

Research Overview: Two plasma models are implemented – the two-fluid 5-moment and the two-fluid 10-moment models which both capture two-fluid effects that are often neglected when using typical single-fluid plasma models. For the 5-moment model, Euler equations with the addition of appropriate Lorentz forces are used to model the ion and electron fluids, while Maxwell equations are used to model the electric and magnetic fields. The 10-moment model expands upon the 5-moment model with the addition of an anisotropic pressure tensor which allows for non-Maxwellian plasma states. The applications shown here are the 3-dimensional Z-pinch using the 5-moment model and the 2-dimensional Harris current sheet using the 5- and 10-moment models. The Z-pinch consists of an axial current that produces an azimuthal magnetic field which balances a radial pressure gradient. The Harris current sheet consists of an in-plane plasma current supporting an out-of-plane magnetic field. The results presented here show the models' abilities to capture solution dynamics at small spatial and temporal scales. These simulations were performed using the *Jaws* supercomputer at Maui High Performance Computing Center.

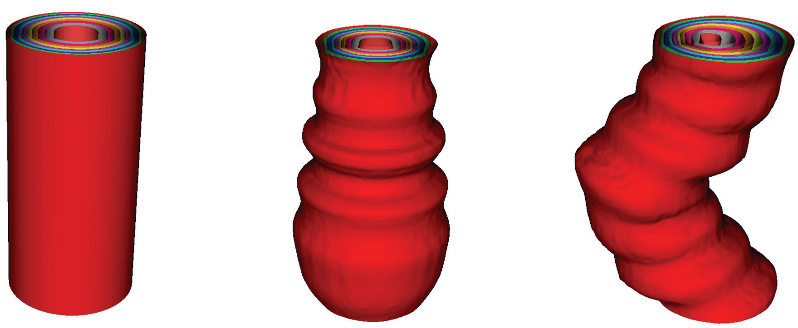

Figure 1. Onset of the lower-hybrid drift instability in a 3-dimensional Z-pinch with initial condition (left), an axisymmetric perturbation (middle) and an asymmetric perturbation (right). Short-wavelength modes form following the initialization of a single wavelength sinusoidal perturbation to the equilibrium profile. The short-wavelength lower-hybrid drift instability requires capturing two-fluid effects. Electron density contours are shown.

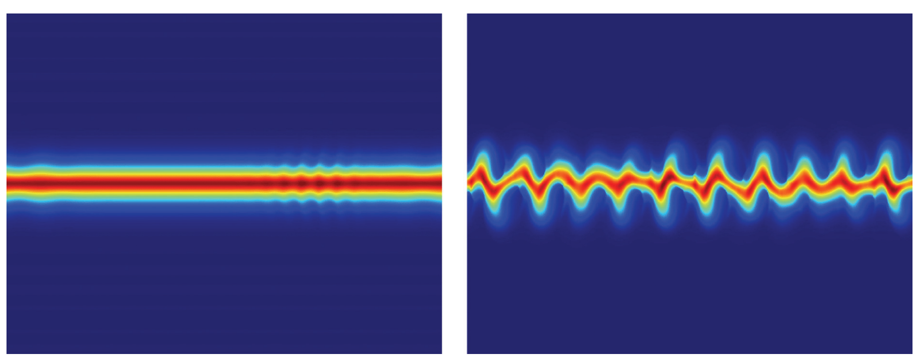

Figure 2. Onset of lower-hybrid drift instability using 5-moment model (left) and 10-moment model with collisions (right) using the same initializations. Short-wavelength modes form following the application of a single wavelength sinusoidal perturbation to the equilibrium profile. Electron density contours are shown.

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Acknowledgement: The authors gratefully acknowledge support for this research from the AFOSR Grant No. FA9550-05-1-0159.

Turbulent Boundary Layers Over Rough Bathymetry

Krishnakumar Rajagopalan and Geno Pawlak

Coral and rocky reefs are characterized by highly irregular and inhomogeneous bathymetry with widely varying roughness scales. The hydrodynamic characteristics for flow over these broad-banded, highly irregular roughness distributions are complex and not well-understood, and the traditional parameterizations and models of such flows are questionable. Nunes and Pawlak (2008)[1] measured roughness over a stretch of coral reef around the Kilo Nalu Observatory and found that the bed was characterized by a broad spectral distribution. We are conducting numerical studies of boundary layer flows over rough beds with this type of broad-banded spectra. The numerical model makes use of large eddy simulation (LES) techniques to solve the partial differential equations governing turbulent fluid flow in the boundary layer. The study is expected to shed light on estimating relevant parameters such as hydrodynamic length scales for turbulent boundary flows over rough bathymetry characterized by spectral roughness.

Introduction: The turbulent processes associated with flow over irregular boundaries such as coral and rocky reefs have important effects on dissipation of wave energy and sediment transport, critical aspects in modeling coastal currents and waves. The *hydrodynamic roughness* scale, z_0 is the critical parameter that relates the physical roughness of the bathymetry and its hydrodynamic response to the flow. In the case of homogeneous roughness traditional methods can be applied to estimate z_0. Nunes and Pawlak (2008)[1] measured roughness over a stretch of coral reef around the Kilo Nalu Observatory and found that the bed was characterized by a broad spectral distribution. We are conducting numerical studies of the turbulent boundary layer over bathymetry which has similar spectral roughness characteristics as that of Nunes and Pawlak (2008).

Methodology: The numerical model uses large eddy simulation (LES) techniques to solve the partial differential equations governing turbulent fluid flow in the boundary layer. LES explicitly solves for the large structures or eddies in the flow that are affected directly by the boundary geometry and models the smaller, near isotropic ones, making it ideal for our application. The computational demands of LES, however, are significantly high, making it suitable only for high performance computing facilities.

Results and Future Work: An important aspect of our work is the generation of bathymetry following the roughness spectrum. Rough bathymetry is characterized by jagged and rough edges where flow separates. A spectrum based on sine waves would be inherently weak in representing sharp corners. Alternately, the spectral roughness can be represented using square waves which may better reproduce flow separation characteristics common to flow over rough beds. Here, we examine both approaches in modeling flow over roughness.

Figure 1 shows vorticity field over a boundary generated from a roughness spectrum using sine waves as basis function. Figure 2 shows the flow over a square block. In both cases the flow separation is clearly visible. The hydrodynamic length scale, z_0 estimated from the mean velocity profiles of the stream-wise velocity averaged over the complete numerical domain, agrees well with other published work. These simulations were carried out to validate the LES solver and to check if the solver computes important hydrodynamic features of the flow. We are currently modeling flow over inhomogeneous, multi-component square waves which represent the broad-banded or inhomogeneous roughness characteristic of reefs. These studies are expected to shed light on bulk parameters of the flow such as mean velocity profile, hydrodynamic length z_0 and bed stress for a boundary with a spectral roughness distribution.

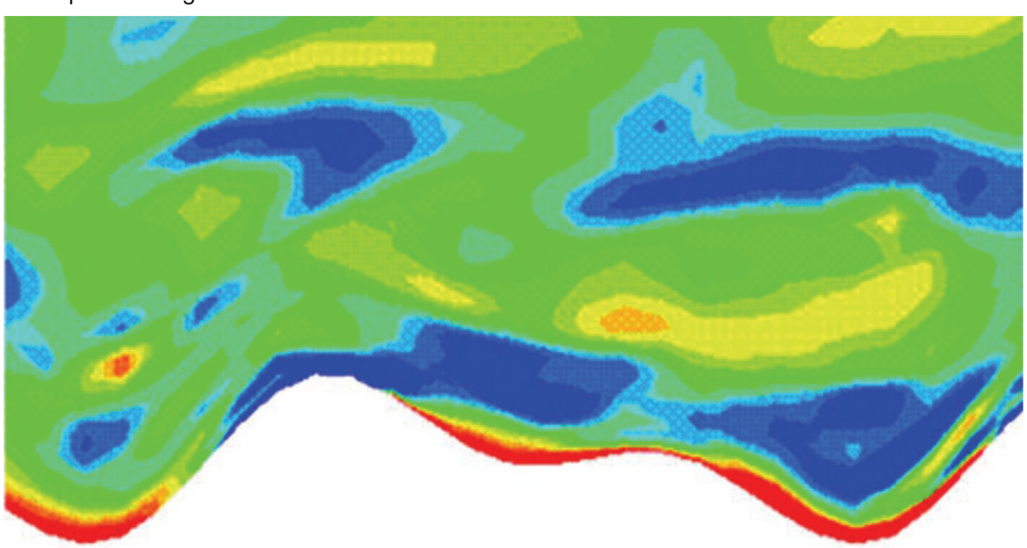

Figure 1. Instantaneous vorticity field over a boundary generated using two sine components scaled following the roughness spectrum of Nunes and Pawlak (2008).

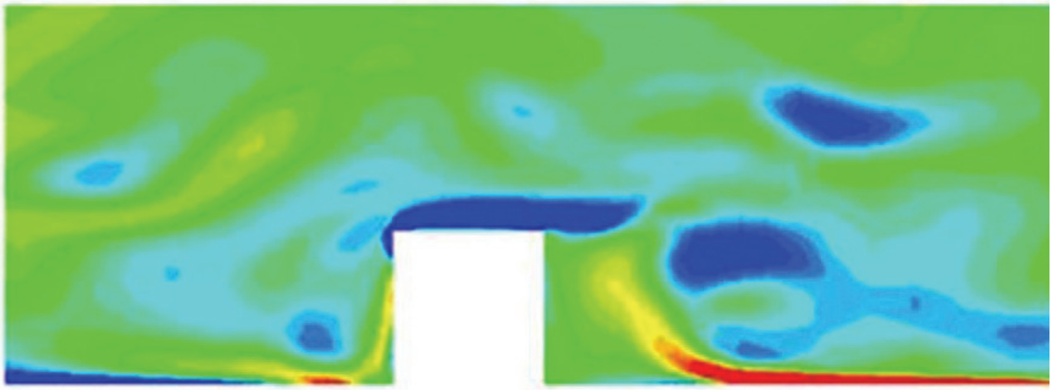

Figure 2. Vorticity field for flow over a single component square rib roughness.

References:

1) Nunes and Pawlak, 2008, "Observations of Bed Roughness of a Coral Reef," *J. Coast. Res.*, 24(2B).

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Acknowledgement: Funding was provided by University of Hawaii through a MHPCC Student Engagement Grant and by the Office of Naval Research.

Training Transformation in the Pacific – Toolkit for Operational Medical Modeling (TOMM)

Robert Dant and Glenda Ramos

TOMM is a decision-support/course-of-action analysis system that allows medical planners and operators to quickly predict the spread and impact of infectious diseases on military forces and resources. An Oracle SOA suite was used to develop an enhanced version of TOMM. An Enterprise Service Bus was used to provide a generic framework for medical data resources to be rapidly made available to any infectious disease models. The Enhanced TOMM System provides detailed analysis of required resources and mission effectiveness impact in preparing for and responding to a Pandemic Influenza outbreak. Additional models can be rapidly integrated into the Enhanced TOMM System based on customer requirements and model availability.

Research Objective: The primary objective was to provide Research and Development (R&D) enhancements for Live, Virtual, and Constructive (LVC) training capabilities in support of PACOM (Pacific Command) Theater-wide training efforts, specifically for the Toolkit for Medical Modeling (TOMM) Program. TOMM is a decision-support/course-of-action analysis system that allows medical planners and operators to quickly predict the spread and impact of infectious diseases on military forces and resources.

Methodology: Research efforts focused on the following:

1. Creating a Service Oriented Architecture (SOA)-based system that pulls data for existing Department of Defense (DoD) Web Services
2. Demonstrating how the SOA enhancements for TOMM could use software components to leverage data and functionality from partner organizations
3. Exposing Web Services having relevant medical or logistical data and demonstrating the technology
4. Automating Simple Object Access Protocol (SOAP) message creation within the TOMM Component Coupler (TCC) which is part of the TOMM Simulation Environment (see Figure 2).

Figure 1. TOMM is a decision support system for medical planners and operators.

We used an Oracle SOA Suite in developing the SOA-based solution for TOMM. This SOA Suite was implemented using a separate machine (laptop) that hosted the Database Server, the Application Server, and the Service Registry. An Oracle JDeveloper was utilized to develop medical data services using JMAR (Joint Medical Assets Repository) data provided by Akimeka, LLC and to interface with the Application Server component of the Oracle SOA Suite. With the SOA-based infrastructure and JMAR data, the medical data sources were made readily available to interface with TOMM. Along with the other components of the Oracle SOA Suite, an Enterprise Service Bus (ESB) was used to provide a generic framework for medical data sources to be readily incorporated and made available to any infectious disease models.

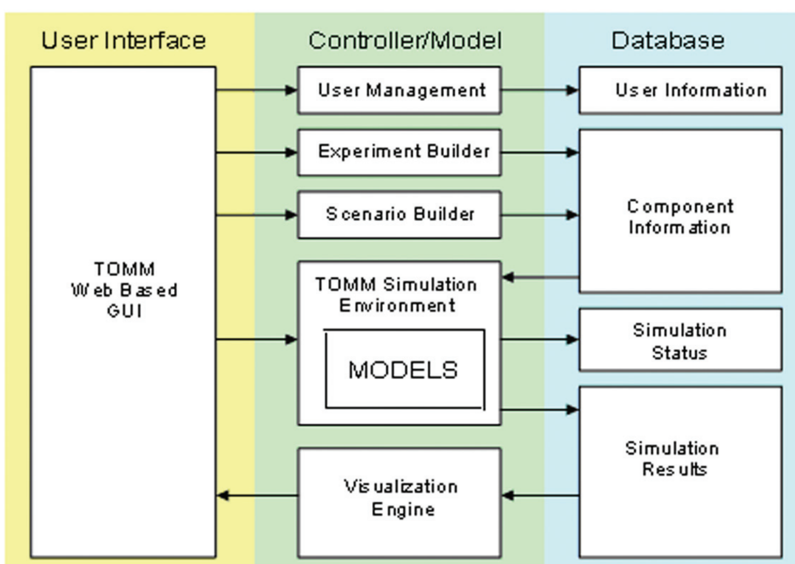

Figure 2. Schematic overview of the TOMM architecture.

Results: We accomplished the following during this research project:

- Worked with PACOM (J81) and Alion Science & Technology (S&T), Inc. to identify requirements for an Enhanced TOMM System having a SOA-based operating environment.
- Investigated the feasibility of using "real" (archived) medical data versus simulated medical data and obtained the use of JMAR data as our source for TOMM Medical Web Services.
- Completed building a SOA-based environment for the TOMM system.
- Developed links to three Web Services that provided medical data regarding Tamiflu, Antibiotics, and Anthrax.
- Utilized the ESB capability of the Oracle SOA Suite as our framework for integrating multiple data sources and exposing them as Web Services.
- Registered three medical Web Services into a Universal Description Discovery and Integration (UDDI) Registry.

THE WAY AHEAD with WEB SERVICES

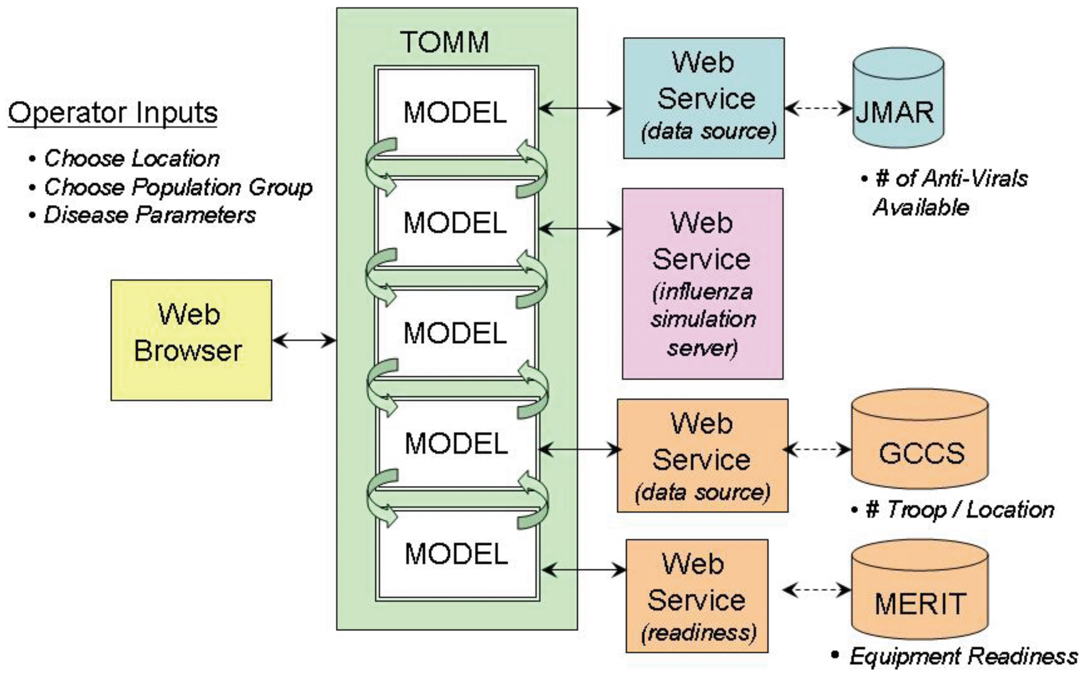

Figure 3. Schematic overview of TOMM applications involving other databases that are accessible via Web Services.

Significance: The Enhanced TOMM System provides detailed analysis of required resources and mission effectiveness impact in preparing for and responding to a Pandemic Influenza outbreak. Additional models can be rapidly integrated into the Enhanced TOMM System based on customer requirements and model availability. Having JMAR data exposed as Web Services on a SOA-based environment significantly improves the likelihood of the same Web Services being used for other medical models. Knowing that these Web Services are registered and available via the UDDI registry, any authorized user can easily obtain the medical information and deliver results quickly through the use of the JMAR Web Services.

Using readily-available medical information, TOMM is now able to accomplish the following:

- Predict the spread of infectious diseases in a more timely manner
- Interoperate with real-world systems
- Rapidly update medical information for course-of-action analysis
- Provide insight into military medical capability and readiness

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Sponsorship: JFCOM and U.S. PACOM
Acknowledgement: Akimeka LLC provided medical data from their Joint Medical Asset Repository (JMAR) resources, which greatly enhanced the validity of this research project.

Finding Seamounts in the Satellite-Derived Gravity Field

Seung-Sep Kim and Paul Wessel

Seamounts are ubiquitous volcanic features on the ocean floor. Understanding their spatial distribution, volumes, and summit depths is important for both practical and scientific endeavors. From a practical perspective, seamounts can pose obstacles to underwater navigation and cause focusing or shadowing of acoustic and tsunami waves. From a scientific perspective, they sustain diverse ecological communities, determine habitats for fish, and act as obstacles to water currents, thus enhancing tidal energy dissipation and ocean mixing. Both geographical- and size-distributions of seamounts give key insight into the variations of underwater volcanism through time and space and the plate tectonic processes that formed them. Therefore, our work involves the development of a nonlinear inversion method for locating and characterizing seamounts from the satellite-derived gravity field.

Research Overview: Despite 50 years of seafloor mapping by research vessels and Navy survey ships, vast areas of the southern ocean basins remain uncharted and hence most seamounts taller than 1 km have not yet been detected. However, the additional gravitational attraction of seamounts (due to their excess mass relative to the surrounding water) causes water to pile up into smooth bumps that perturb the sea surface (i.e., the geoid, an equipotential surface). These bumps have amplitudes of a few meters and length scales of tens to hundreds of kilometer and while ships cannot measure them, orbiting satellites with altimeters can do so easily from space. Processing of satellite altimetry measurements, therefore, can recover anomalous gravity signals over seamounts.[1] In this project, we use the newly released vertical gravity gradient (VGG, or geoid curvature) data derived from satellite altimetry, which provide better spatial resolution than previous data by a factor of two.[2]

As anomalous VGG signals over seamounts may be approximated by either circular or elliptical Gaussians, we can formulate a nonlinear inversion problem that minimizes the difference between our model predictions and observations. The model parameters for the circular Gaussian model are the VGG amplitude and geographical location of the summit, and the basal radius, while the elliptical Gaussian instead needs the major and minor axes of the basal ellipse and the orientation of the major axis. Finally, we impose positivity constraints on the recovered VGG amplitudes and radii using a logarithmic barrier method. The Marquardt method is used for the minimization.[3]

Methodology: In a given area, our method starts searching for seamounts by horizontally slicing the VGG data from top to bottom with a small contour increment (i.e., 1 mGal/km). For a seamount, the polygons resulting from slicing are hierarchically overlapping as the lower slices are larger and contain all the upper ones. If there is another potential seamount nearby, the slicing process will produce another set of overlapping polygons, which eventually become merged with other sets at the lower contour level. Thus, we can construct the initial conditions for the VGG amplitudes and locations of potential seamounts by accumulating the amplitude and location of the first slice whenever a new set of polygons is initialized. Then, using the circular Gaussian model, we visit every potential summit from the highest amplitude to the lowest and test if the inclusion of each summit produces a statistically significant reduction in overall misfit. This decision is accomplished by using the unbiased Akaike Information Criterion (AIC) and an F-test. With the set of statistically significant potential summits, we refine the prediction by testing if an elliptical Gaussian model further reduces the misfit and hence arrive at the most suitable model for all seamounts studied.

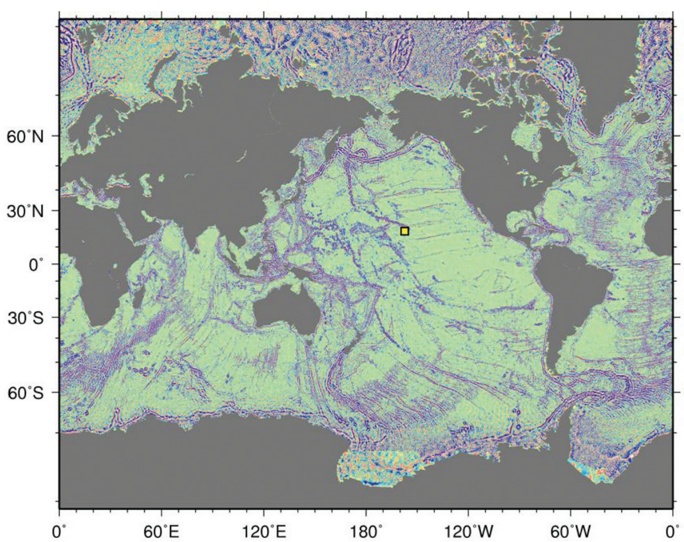

Figure 1. Global map of satellite-derived vertical gravity gradient data. Sea surface heights measured by satellite altimetry approximate the geoid over the ocean. The vertical gravity gradient (VGG) field is the curvature of the geoid and hence obtained by summing the second derivatives of altimetry measurements with respect to the east and north directions.[1] Therefore, seamounts become conspicuous in the VGG field as the derivatives amplify the anomalous gravity signals over them.[4] The yellow square indicates the location of the Geologists Seamount Group where our searching method was tested as shown in Figure 2.

Results: The significance of this study lies on the ability to find seamounts based on the statistical criteria in the presence of noise. In addition, the ability to reconstruct them allows us to investigate relationships between the seamount formation, seafloor age, seafloor fabric and various surrounding tectonic processes. In the near future, this method will be applied to all ocean basins for building a new database of global seamount distribution.

References:

1) Sandwell, D.T. and W.H.F. Smith, "Marine gravity anomaly from Geosat and ERS-1 satellite altimetry," *J. Geophys. Res.*, 1997, 102(B5): p. 10,039-10,054.
2) Sandwell, D.T. and W.H.F. Smith, "Retracking ERS-1 altimeter waveforms for optimal gravity field recovery," *Geophys. J. Int.*, 2005, 163: p. 79-89.
3) Press, W.H., *et al.*, "Numerical recipes in C: the art of scientific computing," 2nd ed. 1992, London: Cambridge Univ. Press.
4) Wessel, P. and S. Lyons, "Distribution of large Pacific seamounts from Geosat/ERS-1: Implications for the history of intraplate volcanism," *J. Geophys. Res.*, 1997, 102(B10): p. 22,459-22,476.

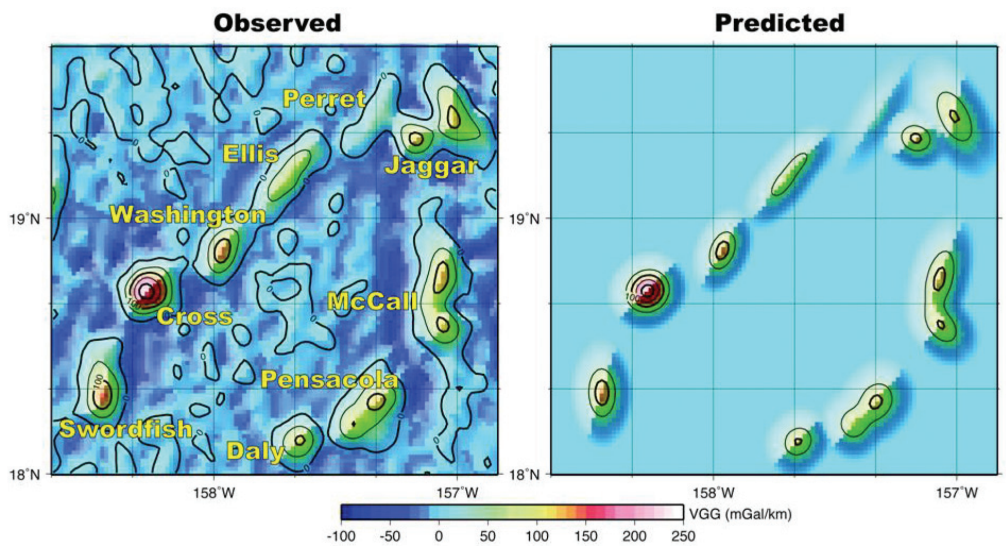

Figure 2. Observed vertical gravity gradient data over the Geologists Seamount Group south-west of the Hawaiian Islands (left) and predicted seamounts (right). The locations and shapes of these known seamounts are well characterized by the nonlinear inversion method developed by this study.

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Sponsorship: Funding was provided by University of Hawaii through a MHPCC Student Engagement Grant.
Acknowledgements: We thank Mary Ann Ciuffini (MHPCC) and Sue Brown (UH) for their prompt assistance with MHPCC resources.

Exploratory Rainfall Simulation of the 2004 Halloween Eve Flash Flood

Guangxia Cao, Duane Stevens, John Porter

This project uses the Weather Research and Forecast (WRF) model to simulate the 2004 Halloween Eve thunderstorm on Oahu, Hawaii. In the late October 2004, an upper level trough hung over the southwest of Hawaii for several days, and triggered the atmospheric disturbances surrounding the Hawaiian Islands. On 30 October 2004, a stronger upper level wind intensified the thunderstorm, and the lower level trades moved the thunderstorms to Oahu, causing the damaging Oahu flash flood. Lack of sufficient meteorological environment information made it impossible for current models to capture this unique event. Our project contributes to the learning of this particular event from a modeling perspective, studying the role of various physics schemes and the modified initial condition for the simulation. The results demonstrated that different model physics regime did have different performances and in this case Betts-Miller-Janjic (BMJ) cumulus parameterization and three microphysics schemes produced the best simulation. Updated model initialization leads to improved case simulation.

Introduction: The fundamental objectives of the numerical weather studies are to correctly predict the extreme weather events in order to assist the forecast mission of property protection for both civilian and military. Model physics and data initialization are believed to be essential for accurate numerical prediction [Kalnay *et al.* 1990].[1] At the present development stage, the initial data become the bottleneck for realizing the potential of weather models. This project uses the 2004 Halloween flash flood as the case, to explore the issue of improving the simulation of heavy rainfall events by focusing on the modification of the initialization data. We used the Weather Research and Forecast (WRF) model, the state of the art model in the operational use, for the exploration. The research has two specific objectives:

i. Test different physical options to identify the best approximation for this case

ii. Modify the initial conditions to identify key initialization strategy for a better forecast or simulation.

Background: In late October 2004, an upper level trough hung over the southwest of Hawaii for several days, and triggered the atmospheric disturbances in the northeast trades flow, generating large areas of thunderstorms northeast of Hawaiian Island. On 30 October 2004, a stronger upper level wind generated vorticity, which intensified the thunderstorm. The lower level trades moved a strip of disturbances from the thunderstorm areas over the Manoa Valley, pouring 283 mm (11.4 inch) of rainfall and causing the damaging Halloween Eve flash flood.

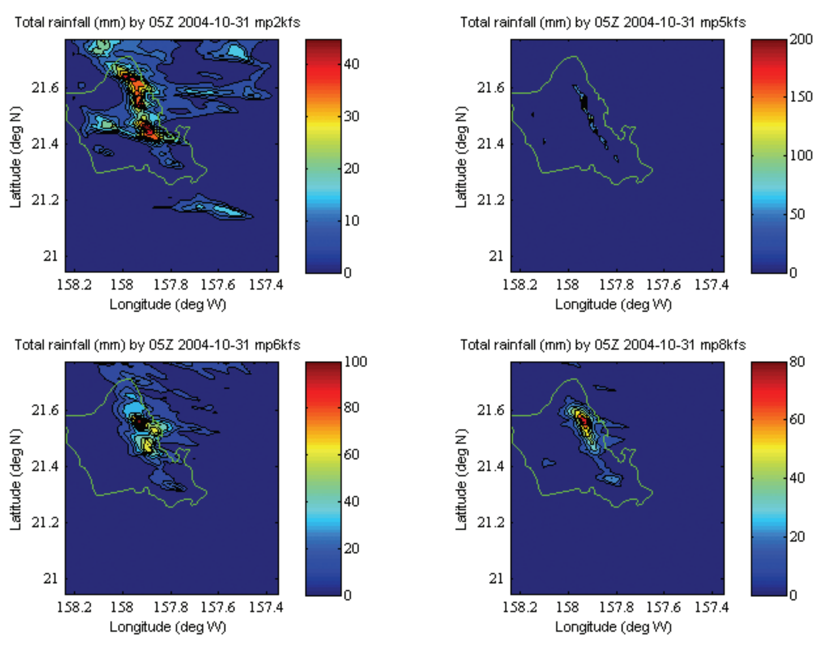

Figure 1. Comparison of 24-hour rainfall simulation (Unit: mm) between four microphysics regimes over Oahu Island, Hawaii. Top left panel: Lin *et al* microphysics, top right: Ferrier microphysics, bottom left: WRF single moment 6 class scheme, and bottom right: Thompson microphysics. These comparisons were made using the Kain-Fritsch cumulus parameterization.

Methodology: The WRF simulation was conducted on the *Jaws* MHPCC, a DELL Linux cluster. We ran the WRF model in three nested domains with the resolutions from 1 to 25 kilometers at a ratio of 5. We used the Global Forecast System data and United States Geological Survey (USGS) topography data to initialize the model, using different initialization time from 00Z 29 Oct. - 00Z 31 Oct. 2004 or in local Hawaiian time 2 pm 28 - 2 pm 30 October 2004.

The WRF model includes three parts: pre-processing (WPS), the WRF core, and visualization (Skamarock *et al* 2008).[2] This project uses the WRF advanced dynamic solver core, i.e., the ARW model. We used WPS to prepare the ARW data, a pseudo-4DVAR approach to change the initial field, and NCAR Command Language (NCL) and Matlab to visualize the model outputs.

The pseudo-4DVAR approach arbitrarily increases the wind shear and air moisture over the vicinity of the Oahu Island in correspondence to the satellite observation. The total simulation time exceeded 32,000 CPU hours, in performing the following comparison runs: dry and wet soils, normal vs. nudging under dry soil condition, normal vs. changed initial field under both dry and wet soil condition, and the modified wind and moisture during the WRF running time.

Results: None of the microphysics schemes correctly simulated the rainfall location (Figure 1), generally the Lin *et al*. microphysics scheme at the top left panel, the WRF single moment 6 class scheme at the bottom left panel, the Thompson microphysics scheme at the bottom right panel produce a wide range of raining area, and the Ferrier microphysics scheme at the top right panel produces the highest rainfall but in a narrow range.

The cumulus comparisons for all microphysics schemes show that the Betts-Miller-Janjic (BMJ) scheme works better, producing higher rainfall. The dry and wet soil simulation results show that the simulation with initial wet soil produces more rainfall. The result from the nudging runs produces a similar pattern as that from the normal runs, indicating that nudging may not improve the forecast or simulation skill for this case. Nudging means that model will conduct the data reanalysis process to smooth out the domain data for improving the simulation.

Modified initial wind field by the pseudo-4DVAR approach and air and soil moisture led to an improved forecast (Figure 2), with a result that the total 24-hour rainfall simulation over Oahu Island is over 300 mm - close to the observation.

Conclusion: In conclusion, this study demonstrated that under the current available model physics, modification of the initialization field is the only approach to achieve the correct simulation of the extreme weather in the Hawaiian region. Given the fact that we have relatively good surface observation in the Hawaiian region, this study suggests that more work should be done on collecting data of the upper level wind to realistically initialize the wind field in the future.

References:

1) Kalnay, E., M. Kanamitsu, and W. Baker, 1990: "Global numerical weather prediction at the national meteorological center," Bulletin of the American Meteorological Society, 71, 1410-1428.
2) Skamarock, W., J. Klemp, J. Dudhia, D.O. Gill, D. Baker, M. Duda, X-Y. Huang, W. Wang, J. Powers, 2008: A Description of the Advanced Research WRF Version 3. NCAR/TN-475+STR, NCAR Technical Note.

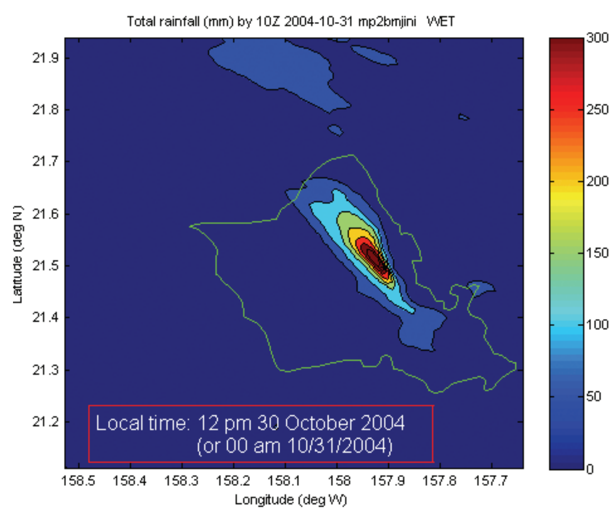

Figure 2. 24 hour rainfall simulation using a pseudo 4DVAR approach. The pseudo 4DVAR approach here artificially increases the wind shear and moisture over Eastern Oahu over 5 hours starting at 00Z 31 October 2004. The Lin *et al.* microphysics and Betts-Miller-Janjic cumulus parameterization were adopted in the simulation.

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Sponsorship: Funding was provided by University of Hawaii through a MHPCC Student Engagement Grant.
Acknowledgement: Thanks to Dr. Sue Brown for administrative and logistics support, Mr. Kevin Roe for the advice on the WRF configuration, and the MHPCC help desk for setting up the WRF model on *Jaws*.

Molecular Dynamics Simulations of a Key Domain of a Connective Tissue Protein

Jhonsen Djajamuliadi, Todd F. Kagawa, Kosuke Ohgo, Kristin K. Kumashiro

Vertebrate tissue has unique lifelong elasticity that is owed to the protein elastin. Elastin is an insoluble polymer that is formed by crosslinking its water-soluble monomer tropoelastin, which, in turn is suitably complex, with over 30 domains. One such domain, expressed by exons 21 and 23, is hypothesized as a critical one for proper folding of the protein and possibly essential for the protein's rubberlike function. The EX21/23 domain of elastin has 33 residues, and the peptide must be studied in water to most closely simulate native conditions. The computational challenges are significant for this 26,000-atom system. Nanoscale molecular dynamics (NAMD), an open-source program intended for implementation with parallel computing, is selected for this problem. The results of these high performance computing (HPC) studies will form the basis of models that may be tested using nuclear magnetic resonance (NMR) spectroscopy and other high-resolution methods.

Research Objectives: The goal of this project is the characterization of the molecular-scale dynamics of a functionally significant peptide found in the connective tissue protein elastin.

Introduction: Elasticity in vertebrate tissues, including skin, lungs, and blood vessels, arises from elastin, the principal component of the elastic fiber. *In vivo*, elastin is assembled from tropoelastin, a multi-domain monomeric protein. The domains encoded by exons 21 and 23 (22 is deleted) has been hypothesized as a critical region for proper folding and elastic function. (Exon 22 is not expressed in humans.) This EX21/23 peptide contains 33 amino acids, of which 5 are the putative hinge residues. Previous studies have shown that the substitution of the hinge with a polyalanine region results in an increased α–helical content and a decreased coacervation temperature.[1] The latter is the temperature-dependent phase transition that occurs in soluble preparations of tropoelastin, so it is often heralded as a mark of a good elastin mimetic. Hence, the physical changes brought on by the "mutations" to the hinge sequence indicate that this region is critical for proper folding of the protein, correct assembly of the fiber (and tissue), and essential for elastic functionality. As with the rest of the native protein, however, limited molecular-scale information, particularly regarding its motion (or *molecular dynamics*), is available for the EX21/23 domain.

The complex nature of elastin presents additional challenges that, in turn, require the powerful resources of high performance computing (HPC). One noteworthy point is the scale of the problem. Elastin must be hydrated for elasticity. Otherwise, it is brittle. For molecular dynamics (MD) simulations, the required computational time increased significantly upon adding the waters of hydration. Hence, the implementation of a parallel computing technique is highly desirable. Nanoscale molecular dynamics (NAMD), "a parallel MD code designed for high performance of large biomolecular systems,"[2] is hence selected as an ideal tool to solve this problem. Simulations of the water-solvated EX21/23 peptide of human elastin were performed on the *Hurricane* cluster at the Maui High Performance Computing Center (MHPCC).

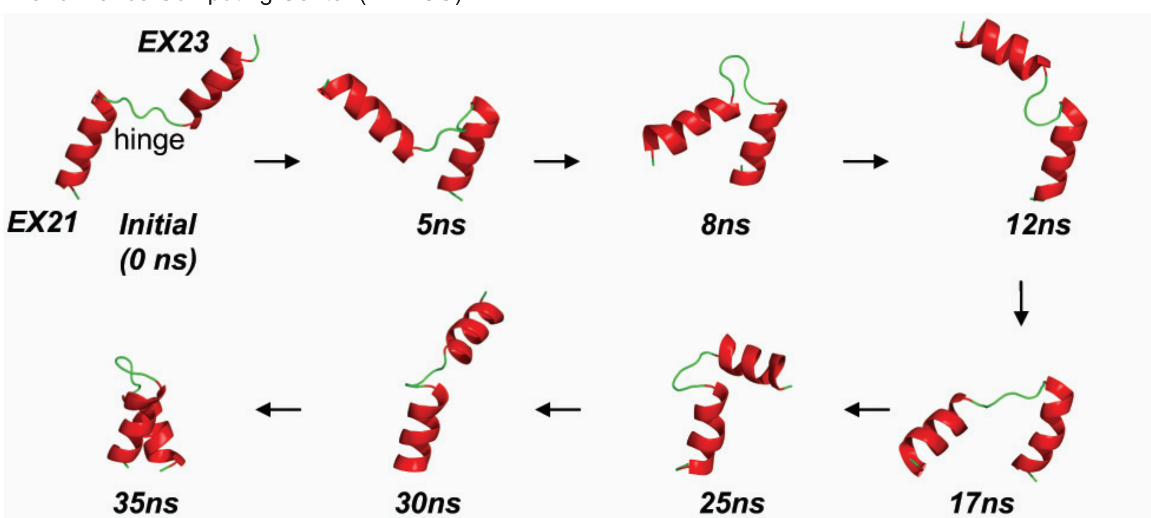

Figure 1. Representative structures of the elastin model peptide at selected time points in the MD simulation. Structures reflect hinge flexibility and variations of relative helical orientations. For comparison purposes, the orientation of the helix of EX21 is fixed in this illustration, and no water atoms are displayed.

Methodology: Initial structural parameters for the EX21/23 peptide use an overall conformation of (α-helix)-(hinge)-(α-helix). The coordinates of the 5-residue "hinge" were built using solved PDB structures that were identified with a BLAST[3] search for short-near-exact matches. The NAMD[2] package was used to run the MD simulation, and VMD[4] was adopted for visualization and performing the analysis. Each homology model was simulated in water at 300K, using periodic boundary conditions and the explicit atom representation. The 33-residue protein was solvated in a (65 x 65 x 65)Å water box, for a total of ~26,000 atoms. MD simulations were performed on the *Hurricane* IBM SP cluster at the MHPCC.

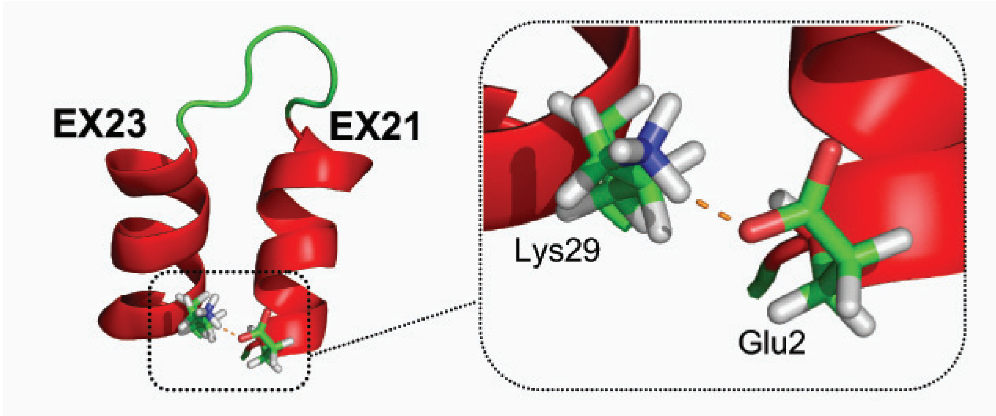

Figure 2. Ribbon structure of a converged structure with folded or “closed” geometry. The overall conformation is stabilized by a salt bridge that has formed between Glu-2 (EX21) and Lys-29 (EX23) residues.

Results and Significance: The NAMD-based approach is intended specifically for parallel computing, optimizing efficiency while providing a physically rigorous computational environment for the study of peptide dynamics. The limit of NAMD parallelization scale is estimated to be about 1000 atoms per processor for good efficiency.[2] At MHPCC, MD calculations on our 26,000-atom system of peptide and solvating water molecules were carried out on 32 processors of the IBM SP cluster. Additional processors increased the computational time only slightly. After energy minimization of the starting structure, molecular dynamics simulations were done. A new structure was calculated at every 10 ps of the dynamics run, to produce a 50 ns trajectory. I.e., for an MD "run" occurring for 50 ns, 5000 structures were calculated and analyzed. The performance benchmark of NAMD on a 32-processor IBM SP cluster was 8.9 hours per nanosecond of simulation. This rate was (almost 32 times) faster than a single-processor desktop computer performing at 281 hours per nanosecond of simulation.

The MD simulations provided information on the motions of the residues and the overall conformation during the 50 ns total time period, as well as structural details of the converged structure. i.e., independent of the starting conformation, the EX21/23 peptide settles into a minimum that is characterized by a compact hairpin structure. From that point, there was very little change in the structure and dynamics of the peptide. In the initial period of the 50 ns run, the peptides exhibit flexibility that originates from the central hinge region. Such flexibility allows the two α-helical regions to access a large segment of conformational space, as shown in Figure 1. After convergence, the torsion angle distributions found for the hinge residues suggest that, esp., glycines and the proline adopt more than one conformation. These computations also reveal striking similarities in the converged structures, most notably the salt bridge formed between the termini, as illustrated in Figure 2.

MD simulations on the MHPCC cluster were invaluable for characterizing the motions of this peptide. In addition, all starting structures converged to a similar, compact form, allowing some analysis of structure, as well as dynamics. These studies could not have been completed in a reasonable timeframe on single- or dual-processor desktop computers.

References:

1) Miao, M., Cirulis, J.T., Lee, S., and Keeley, F.W. (2005), “Structural determinants of crosslinking and hydrophobic domains for self assembly of elastin like polypeptides,” *Biochemistry* 44:14367-14375.
2) Phillips, J.C., Braun, R., Wang, W., Gumbart, J., Tajkhorshid, E., Villa, E., Chipot, C., Skeel, R.D., Kale, L., and Schulten, K. (2005), “Scalable molecular dynamics with NAMD,” *Journal of Computational Chemistry*, 26:1781-1802. “NAMD was developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign.”
3) Altschul, S.F., Madden, T.L., Schaffer, A.A., Zhang, J., Zhang, Z., Miller, W., and Lipman, D.J. (1997), “Gapped BLAST and PSI-BLAST: a new generation of protein database search programs,” *Nucleic Acids* Res. 25:3389-3402.
4) Humphrey, W., Dalke, A., and Schulten, K., (1996),“VMD - Visual Molecular Dynamics,” *J. Molec. Graphics,* 14:33-38.

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The Unmanned Systems Test Bed (USTB)

Robert Dant and Matt Burnham

The U.S. military services are evolving their war fighting systems with an increasing emphasis on unmanned vehicles. Although the trend began with intelligence, surveillance, and reconnaissance (ISR) assets, it is evolving to include combat vehicles and utility platforms. The evolving network-centric warfare concepts of all services increasingly rely on unmanned platforms. The Central Test & Evaluation Investment Program (CTEIP) is interested in finding effective uses of UAV visualization software. CTEIP also wants to leverage TENA (Test & Training Enabling Architecture) for cross-range and cross-facility interoperability. TENA is heavily used by the Test and Evaluation community and UAVs commonly use CoT events for interoperability. The CoTGateway developed by MHPCC is a significant capability for translating CoT events to and from TENA.

Research Objective: The primary objective of the Unmanned Systems Test Bed (USTB) program is to develop new training, test, and evaluation concepts and capabilities for unmanned systems and to conduct a series of demonstrations.

The program sponsor, the Central Test & Evaluation Investment Program (CTEIP) examines how to augment DOD Test and Training Range resources with new capabilities in support of unmanned systems. CTEIP is particularly interested in finding effective uses for visualization software to support the capabilities of unmanned systems. Related goals include leveraging the Test and Training Enabling Architecture (TENA) for cross-range and cross-facility interoperability.

Methodology: The key concept behind this test bed is to integrate Live, Virtual and Constructive (LVC) entities (i.e., troops, vehicles, etc.), including unmanned systems, into a synthetic environment to create an augmented environment to support various test, evaluation, and training scenarios. One important part of integrating unmanned systems is to use any sensor data as part of this augmented synthetic environment.

Results: In order to evaluate the validity of integrating unmanned systems into synthetic environments that combined LVC entities, the USTB program was used for several demos and expos. While TENA is heavily used in the Test and Evaluation (T&E) community, unmanned systems commonly use Cursor on Target (CoT) events for interoperability. To support these exercises, the USTB components were the CoT Gateway, Scene Generator,and Unmanned Air Vehicle (UAV) emulator (see Figure 1).

Cursor on Target (CoT) Gateway - CoT is an emerging standard DoD messaging system used for the exchange of "What, Where and When" tactical information. The CoT gateway was used to translate CoT events to and from TENA.

UAV Emulator - Many times, live UAVs are not available and even when they are available, the data they produce can be error prone due to latency, update rates, wind, etc. A UAV emulator was developed to produce CoT events that can be used as if they were being produced by a live UAV. This emulator has the ability to fly around a synthetic environment and capture sensor frames that are then published as CoT events.

Scene Generator - This is a stealth viewer that renders the synthetic environment. This includes the synthetic terrain, LVC entities, and sensor video streams projected onto the synthetic terrain.

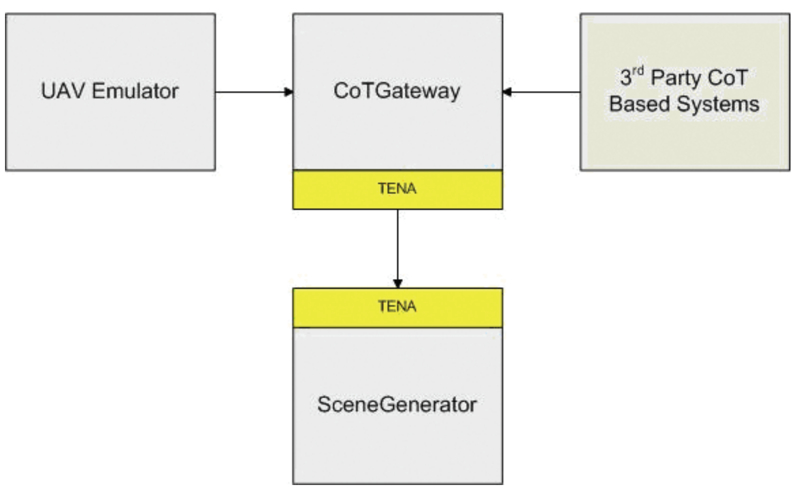

Figure 1. This figure illustrates the USTB components used to verify and validate the integration of CoT and TENA-based systems.

Significance: The U.S. military services are evolving their war fighting systems with an increasing emphasis on unmanned vehicles (see Figure 2). Although the trend began with intelligence, surveillance, and reconnaissance (ISR) assets, it is evolving to include combat vehicles and utility platforms. The evolving network-centric warfare concepts of all services increasingly rely on unmanned platforms. The associated command, control, communications, computers, intelligence, surveillance, and reconnaissance (C4ISR) systems are adopting interoperability standards that include unmanned systems. It is increasingly more important for the individual services and the Joint Commands to develop concepts and facilities for training exercises, CONOPS development, and system T&E which include unmanned vehicle operations. Although much of this will be accomplished in distributed exercises involving computer-generated virtual environments and simulation, it must also include live exercise components on a test range that provides for air, ground, sea-surface, and underwater unmanned vehicle operations.

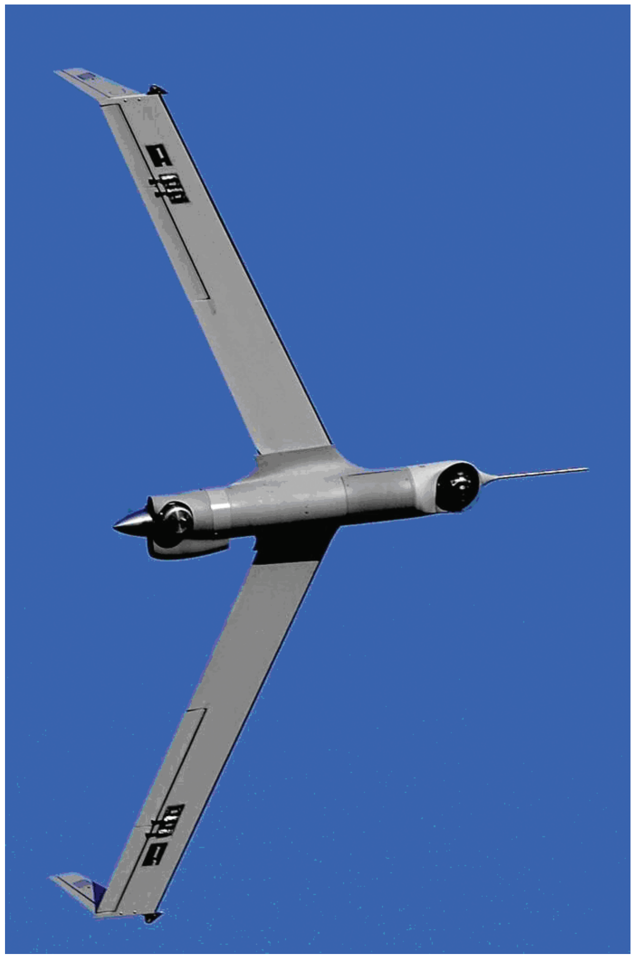

Figure 2. Boeing's Scan Eagle UAV.

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High Performance Computing Software Applications for Space Situational Awareness

Bruce Duncan

The High Performance Computing Software Applications Institute for Space Situational Awareness (HSAI-SSA) has completed another year of applications software development, continuing its work upon competitive selection in government fiscal year 2005. Work this year has been performed on ten sub-projects.

HSAI-SSA coordinates directly with the research, development, acquisition, and operations and support communities to develop and transition HPC software applications, striving to provide game-changing SSA capabilities. The effort performed by the Institute is overseen by the HPCMP Director, who chairs a Board of Directors which is comprised of other senior Department of Defense/SES/General Officer officials.

This paper focuses on work performed during this year to continue improving space surveillance sensor model and image enhancement software. These applications include the Space Surveillance Network Analysis Model (SSNAM), Physically Constrained Iterative Deconvolution (PCID) image processing software, and Advanced Speckle Imaging Reconstruction Environment (ASPIRE) software. The software applications improvements that the HSAI-SSA has made is continuing to have substantial impact to the warfighter and is expanding the role of high performance computing in SSA.

Introduction: The mission of the High Performance Computing Software Applications Institute for Space Situational Awareness (HSAI-SSA) is to support SSA needs of stakeholders by developing High Performance Computing (HPC) software applications for SSA. The Institute collaborates directly with experts and end users in the Joint Space Control mission area in order to identify those "leverage points" at which HPC can be applied to make a strategic difference in how the mission is performed. The HSAI-SSA has had a successful period of performance thus far during this past year, working with multiple software applications, three of which are highlighted below.

Project Updates: Project Updates: HSAI-SSA work has continued, including further development of three software applications: with one responding to Strategic Goal 1 (Astrodynamics) objectives, and two responding to Strategic Goal 2 (Image Enhancement) objectives. All applications continue to run on the Maui High Performance Computing Center (MHPCC) Cray XD-1 Linux supercluster named Hoku (star in the Hawaiian language). The Space SSNAM application is used by Air Force Space Command to analyze the performance of the global space tracking network, or SSN, and is being re-engineered to run as a scalable parallel process while also implementing Special Perturbations (SP) processing. The PCID image enhancement software and ASPIRE tool for space surveillance have also been continually optimized for faster, more precise operations.

The original version of the Space Surveillance Network Analysis Model (SSNAM), which previously used less accurate General Perturbations (GP) satellite orbit propagation, was improved and placed into operation at MHPCC two years ago. During the past year, the SSNAM software architecture was updated and work on the speedup and parallelization of the Special Perturbations (SP) Tasker portion of this software (this is the same software used daily by the Air Force for tasking of space surveillance network sensors to aid maintenance of the satellite catalog) for higher precision SP processing was performed. SSNAM presently is comprised of more than 1,100,000 source lines of code (including Fortran, Java, C, and C++) with approximately 7,000 files. The porting of SSNAM and implementation at MHPCC have proved beneficial to the SSNAM user community, and the integration of SP processing has improved confidence in the accuracy of the solutions generated by SSNAM. Software engineering has resulted in the decreased overhead of SP processing, enabling the use of a higher number of processors to be utilized for SSNAM processing to decrease run times.

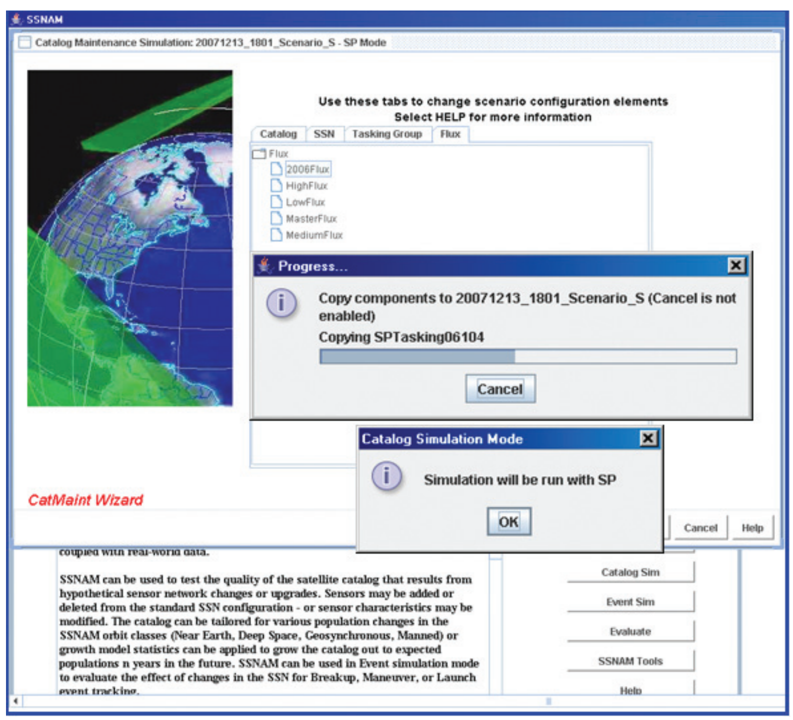

Figure 1. SSNAM software tool SP mode processing graphical user interface is used to launch SSNAM model runs that utilized high precision Special Perturbations (SP) processing.

Figure 2. The ASPIRE graphical user interface tool is used for various functions including to view, store, and manage space object image processing recoveries, such as those generated by PCID image processing software.

Physically Constrained Iterative Deconvolution (PCID) image processing software engineering work and successes achieved during the past year with the latest version of PCID have resulted in further increased efficiency of this code. PCID is currently comprised of more than 15,000 source lines of code (Fortran and C++) with 54 files. An optimized version of the Numerical Recipes conjugate gradient routine has been developed, implemented, and tested. Results obtained and analysis performed thus far using the same space object, data set, and identical parameters have shown that PCID is faster using an optimized Numerical Recipes conjugate gradient minimizer than another available image processing code and technique. The PCID team has also determined that PCID execution with spatial Point Spread Function (PSF) estimation using Gaussian plus Poisson weighting is better than PSF estimation using Zernike with Poisson weighting.

HSAI-SSA work was also performed this year on the next release of the Advanced Speckle Imaging Reconstruction Environment (ASPIRE) software. ASPIRE is a Web-based graphical user interface, job submission, analysis, and data management application that supports the execution of various image processing software applications, including PCID. The current version of ASPIRE is comprised of more than 62,500 source lines of code. This includes a mix of Scripts comprised of Dynamic Java, C, Shell Scripts, and Perl. It also includes Web software comprised of HTML, CFML, Dynamic Java Servlets, CGI, PHP, Cascading Style Sheets, and JavaScript. The HSAI-SSA team has continued to make excellent progress on ASPIRE, including expansion of image processing job submission, monitoring, and management functions. Work during the summer time frame continued, resulting in the completion of testing and identifying, reporting, and resolving issues brought up in the sustained ASPIRE development testing regimen. During late summer, the ASPIRE team work was focused on implementation, flow, integration, validation, layout, and JavaScript support. The final remaining tasks also included completion of a quick turnaround preview capability to view raw image files, select a frame and parameters, create ensembles, compute the package, view results, and improve the ease of use to repeat this operation cycle. Efforts were also applied to rearrange the job submission form layout, modify the submit wrapper backend, automate the output Flexible Image Transport System (FITS) viewing, and complete an enhanced raw file frame selection tool. A thumbnail capability allows for more insight, enhanced selection capability, and to display frame information details per frame. After all of this is completed, the team plans to release the ASPIRE tool to image analysts for added evaluation.

Conclusion: Through sustained funding, software engineering, and technical successes, the HSAI-SSA has continued making significant progress in developing HPC SSA applications for the warfighter. The team has been able to build on the order of magnitude speed-ups in space surveillance models and image enhancement software that have been previously achieved. The HSAI-SSA has continuously employed proven and improved software development and engineering practices to demonstrate performance and/or scalability improvements. HSAI-SSA is focused and bringing the appropriate technical expertise together with the right computing resources and techniques to develop, test, and transition HPC software applications into the critical SSA arena.

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Acknowledgements: The author expresses additional thanks to the Air Force Research Laboratory's Directed Energy Directorate; Air Force Maui Optical & Supercomputing Site; HSAI-SSA Onsite Director, staff, and associates/partners; and the MHPCC contractor team.

High-Resolution Forecasts to Support AMOS Using WRF

Kevin Roe

The Hawaiian Islands contain a variety of microclimates in a very small region. Some islands have rainforests within a few miles of deserts; some have 10,000 feet summits only a few miles away from the coastline. Because of this, weather models must be run at a much finer resolution to accurately predict in these regions. The Weather Research and Forecasting (WRF)[1,2,3] modeling system (version 2.2) is run from a coarse 54 km horizontal resolution (surrounding an area of approximately 7000 by 7000 km) nested down to a 2 km horizontal resolution (and 55 vertical levels) daily. Since the computational requirements are high to accomplish this in a reasonable time frame WRF is run in parallel on MHPCC's Cray Opteron cluster. Utilizing 32 nodes (2 processors per node) the WRF model is run daily over the above conditions in under 4 hours for a 48 hour simulation. Although these forecasts are relatively new, over seven years of numerical weather simulation experience with MM5 and RSM have contributed to its effective use. Operators at the telescope on Haleakala, Maui, utilize this WRF simulation in their daily planning.

Research Objectives: The telescope operations on Haleakala are highly dependent on weather conditions on the Hawaiian Island of Maui. If the wind speed is too high then the telescope cannot be utilized. Problems also exist if there are clouds overhead. Rainfall and relative humidity are also a factor in determining the capabilities of the telescopes. Lastly, optical turbulence (or "seeing") is predicted over Haleakala using the output conditions from WRF.[4] In order to effectively schedule telescope operations, an accurate weather prediction is extremely valuable. Current forecasts that are available from the National Weather Service (NWS) give good indications of approaching storm fronts but only at a coarser level (10-12 km resolution), which can be insufficient for the operators of the telescopes. The additional benefit of the telescope operators having access to an accurate forecast (even for only a day in advance) is that they can still perform some scheduling. If a storm is predicted they can plan maintenance for this time period. This allows them to function more effectively by giving them the capability to schedule downtime. This in turn saves time, improves operating efficiency, and potentially saves money.

Daily Operations: Every night at Midnight Hawaiian Standard Time (HST), a PERL script is run to handle all the operations necessary to produce a forecast on MHPCC supercomputers, prepare images of weather fields (wind, temperature, relative humidity, rainfall, CN^2, etc.), and post it to the MHPCC web page (http://weather.mhpcc.edu).

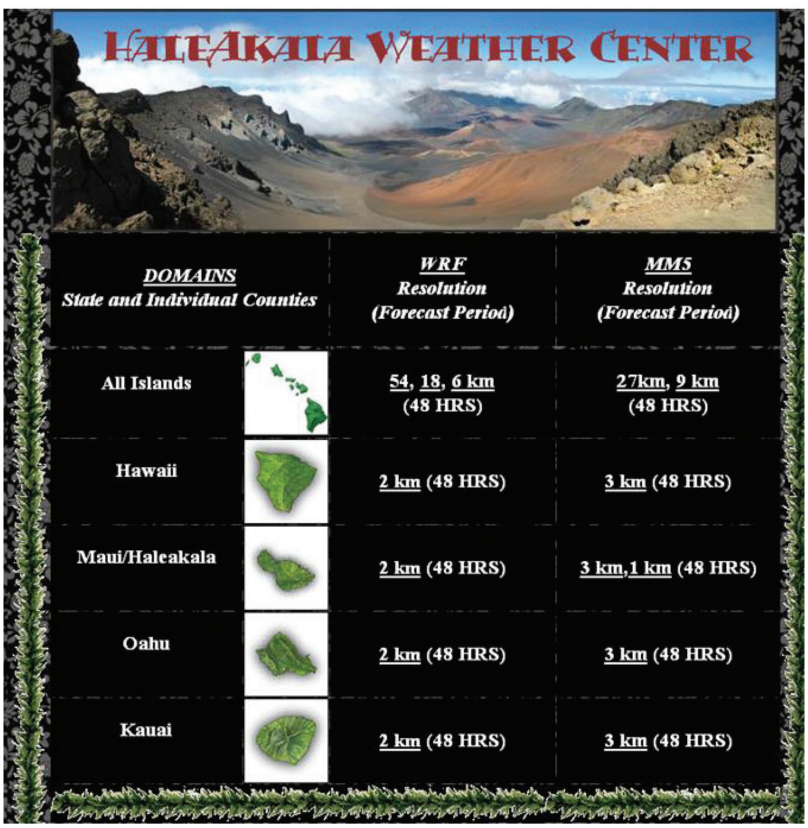

Figure 1. Haleakala Weather Center Homepage.

Web Output: Now that the above processes have created images, they must be made available for the telescope operators. This is accomplished by posting the images to the MHPCC web page; specifically, http://weather.mhpcc.edu. This title page gives the user the option to select the area and resolution they would like to examine. From the title page, the user can select the all island area at a 54, 18, or 6 km resolution or 1 of the 4 counties (Hawaii, Maui, Oahu, and Kauai) at a 2 km resolution. Once one of the above has been selected, the user is transported to a web page that initially includes an image of the wind in the selected area. On this regional web page, the viewer can select to see the previous or next image through the use of a small JavaScript. If the viewer prefers, an animation of the images (in 1 hour increments) can be started and stopped. Finally, the user can select any of the other images from a pull down menu. If the viewer would like to change the field being examined, a pull down menu on the left side of the page will transport the user back to the main menu, a different county, or allow them to choose a different weather field.

References:

1) Michalakes, J., J. Dudhia, D. Gill, T. Henderson, J. Klemp, W. Skamarock, and W. Wang: "The Weather Research and Forecast Model: Software Architecture and Performance," Proceedings of the Eleventh ECMWF Workshop on the Use of High Performance Computing in Meteorology Eds, Walter Zwieflhofer and George Mozdzynski, World Scientific, 2005, pp 156-168.
2) Michalakes, J., S. Chen, J. Dudhia, L. Hart, J. Klemp, J. Middlecoff, and W. Skamarock: Development of a Next Generation Regional Weather Research and Forecast Model, "Developments in Teracomputing: Proceedings of the Ninth ECMWF Workshop on the Use of High Performance Computing in Meteorology Eds," Walter Zwieflhofer and Norbert Kreitz, World Scientific, 2001, pp. 269-276.
3) Skamarock, W. C., J. B. Klemp, J. Dudhia, D. O. Gill, D. M. Barker, W. Wang, and J. G. Powers, 2005: A description of the Advanced Research WRF Version 2, NCAR Tech Notes-468+STR.
4) Ruggiero, F., Roe, K. P., DeBenedicts, D.A., "Comparison of WRF versus MM5 for Optical Turbulence Prediction," DoD High Performance Computing Modernization Program User Group Conference, Williamsburg, VA, 2004.

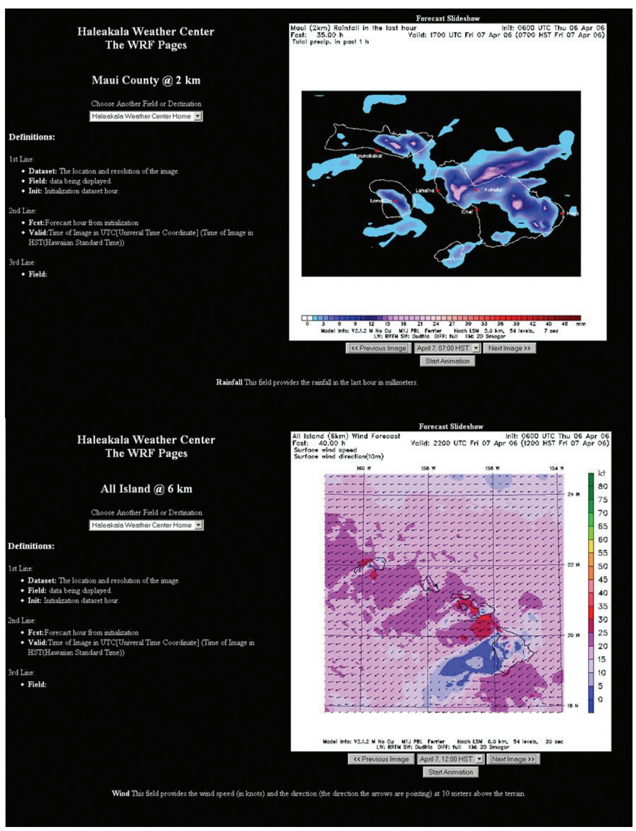

Figure 2. Examples of weather conditions such as rainfall and surface wind speed and direction.

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On the Cover: The snapshot on the cover is a Computational Fluid Dynamics simulation of the F16 - C, at Mach = 0.6, 5,000 ft., 25^{o} angle of attack, vorticity iso-surface (1,000/sec.), and colored by pressure (psi). This project utilized nearly two million CPU hours during FY08 on the Dell PowerEdge cluster, Jaws, at MHPCC. This image was provided by the Principal Investigators: Keith Bergeron, Scott Morton, Dave McDaniel, and John Dean. The Project was sponsored by the DoD HPCMP Challenge Projects (*High Resolution Simulation of Full Aircraft Control at Flight Reynolds Numbers*), the USAF Academy, and the AFRL Directed Energy Directorate.

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