

Call for PETTT Program Pre-planned Project Concept Proposals

General Guidance and Instructions for KY06 Proposal Submission

Introduction

The Department of Defense (DoD) High Performance Computing Modernization Program Office (HPCMPO) sponsors the User Productivity Enhancement, Technology Transfer and Training (PETTT) Program for the benefit of DoD Service/Agency high performance computing (HPC) users in executing their missions. The HPCMP is administered and executed by the Army Engineer Research and Development Center (ERDC), Vicksburg, MS. The objective of PETTT is to enhance DoD HPC user productivity by providing world-class technical support and training through strategic partnerships and focused enabling tool development and deployment. The PETTT program is responsible for gathering and deploying the best ideas, algorithms, and software tools emerging from the national HPC infrastructure for the DoD user community.

In support of this program, the HPCMPO funds pre-planned projects that are intended to improve the usability, effectiveness and impactfulness of HPC resources or extend their use into new domains or address new problems. Pre-planned projects may include:

- Cooperative software research and development of DoD mission applications involving HPC systems.
- Software application performance assessments and performance tuning for HPC systems.
- Development of software tools for use across the HPC community.

Pre-planned projects should positively impact one or more Service acquisition or warfighter programs or a broad base of DoD HPC users. They may also provide benefits by:

- Supporting multiple DoD services
- Contributing special expertise to HPCMPO projects (e.g. CREATE, Institutes, etc.)
- Leveraging existing funding from DoD or other agencies.

All PETTT pre-planned projects must be initiated by the DoD Government scientist/engineer sponsor requiring HPC resources to enhance mission productivity. The terms sponsor, stakeholder and user are synonymous in the context of this guidance. All projects will be funded and executed by subcontractors through the PETTT contract.

Pre-planned projects are developed in a two-step process: the first step is the submission of a Concept Proposal by the DoD Government Sponsor (format described below) and the second step is the submission of a Full Proposal, by a Contractor/ Principal Investigator (PI). The DoD Government sponsor, jointly with the PETTT prime contractor, has the responsibility to monitor and oversee technical progress and timeliness of project execution. The DoD Government sponsor must be a civil servant or IPA and the Project PI must be an industry or academic institution contractor.

In preparation for Contract Year 6 (KY06) (September 1, 2014 – August 31, 2015), this call is being issued to identify concepts for projects to be executed in KY05. Computational

Technology Area (CTA) trends and challenges that are of critical interest to the program have been identified and are attached as an appendix (each trend and challenge has an identifier associated with it that begins with **TC-**). Responses should explain how the project would address one or more of these trends and challenges and how the project would positively impact one or more Service acquisition or warfighter programs or a broad base of DoD HPC users. Proposals should also indicate the expected length of the project and whether the project is expected to be a small (<\$75K) or large (\$75K-120K) effort.

Guidelines for Concept Proposal Preparation

Those interested in submitting a TWO PAGE concept proposal should provide the following information using the attached template:

- Suggested Project title
- Recommended [Contractor/Academic] Principal Investigator (if known – if required PETTT can assist in identifying a PI for selected concept proposals)
- Expected pre-planned project duration and size
- Contact information for the Primary DoD user/sponsor (i.e. the project's principal point-of-contact for the user base) and Secondary DoD users/sponsors
- Recommended Primary Computational Technical Area (CTA) and Associated CTAs.
- Description of the DoD need being addressed and the expected impact to one or more DoD R&D objectives in basic science, applied science, and/or special capabilities ***through the use of HPC*** and/or ***development of new HPC technologies*** to advance the overall HPCMP mission. This should include identification of the specific trends and challenges that will be addressed and how this will benefit the DoD and/or the HPC community.
- Overview of the technical approach
- Identification of anticipated deliverables.

This section should be no more than 2 pages, 12 pt Times New Roman font and Single Spacing format.

Concept proposal applicants are encouraged to use and demonstrate 'lessons learned' with other HPCMP Initiatives. These lessons will be incorporated into providing a better suite of services as this technology is deployed to the various sites/Centers.

Submission of Concept Proposals

All concept proposal submissions must be at an unclassified level. Do not include any controlled or sensitive information. Using the attached template, the DoD Government sponsor should submit the concept proposal to pettt_projects@drc.com by March 17, 2014. Questions regarding this call should be directed to pettt_projects@drc.com.

Next Step: Full Proposals

If the concept proposal is selected for further consideration, a detailed full proposal for the project will be requested from a Contractor Principal Investigator. The Government Sponsor

will be asked to review this full proposal and to provide a supporting statement attesting to the importance and priority of the proposed work and expressing how this proposed activity will enhance and contribute to the users' work. The sponsor will also be asked for a commitment to review the project deliverables presented for acceptance. The detailed full proposals will be evaluated on technical excellence, as well as other criteria which will be provided in the call. Selected projects will be prioritized for award as funding becomes available.

Appendix. Computational Technology Area (CTA)-Technical Trends and Challenges

Table 1. Computational Technology Area (CTA)-Identified Trends and Challenges

| CTA | Trends and Challenges (CTAs involved) |
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| ENS | <p data-bbox="297 239 873 268">Electronics, Networking, and Systems/C4I</p> <ol style="list-style-type: none"> <li data-bbox="345 275 1369 743"> <p>1. TC-ENS1 - DoD mission requirements increasingly drive RD&E efforts to explore deployable HPC solutions, as opposed to the traditional model of HPC center with reach-back capabilities. This trend is driven by the perception that new technologies (e.g., general-purpose graphics processing units or GPGPUs), can enable new capabilities qualitatively different from those previously accessible near or within a theater of operation. The approach resolves the challenge of applying HPC technology to direct mission requirements, which has historically not been resolved in a meaningful way. The challenges posed include the research and development for hardware systems and software for mission planning, C4I (command, control, computing, communication and intelligence), situational awareness applications in support of direct mission requirements, and electronic warfare applications. (ENS)</p> <li data-bbox="345 764 1369 978"> <p>2. TC-ENS2 - Large-scale network simulation and emulation for the study of military communication systems including physical effects for voice/video/data networks, is of high interest and importance for the DoD, as such systems will form a critical component of future strategic and tactical systems. Such systems include, but are not limited to, mobile ad-hoc networks (MANETs). (ENS)</p> <li data-bbox="345 999 1369 1251"> <p>3. TC-ENS3 – The growth rate of data per DoD sensor platform and the number of such platforms is increasing rapidly resulting in processing bottlenecks at both the aggregation point for in-theater data streams and within analyst workflows. The ENS challenge is to leverage HPC technology, including the use of hardware accelerators, and techniques to accelerate C4I workflows for analysts confronting this ever increasing volume of sensor data. (ENS)</p> <li data-bbox="345 1272 1369 1671"> <p>4. TC-ENS4 - An emerging shift in the design of processor technology for high throughput, technical and high-performance computing will have a significant impact on the systems available to support DoD requirements. This shift includes hybrid multi-core and/or low-power (CPU)/many-core (GPU) architectures, and the use of other accelerators and with massive on-die parallelism. These architectures have already taken the top positions on the HPC Top 500 lists, a trend that is expected to continue. The challenges associated with this trend include system architectures, software porting, design, development and optimization, and the identification of new opportunities for the application of HPC technology for DoD mission requirements. (ENS, Cross-CTA)</p> <li data-bbox="345 1692 1369 1902"> <p>5. TC-ENS5 – This task supports multi-scale modeling of electronic and photonic devices and circuits in support of RD&E activities that develop next generation military systems containing these devices as critical components. For several decades, the modeling and design of electronic components relied upon model reduction to enable reasonable time-to-solution metrics. With the semiconductor industry rapidly approaching</p> |

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| | <p>technology nodes that introduce physical effects qualitatively more challenging than those previously confronted, the industry has recognized the need for combined multi-scale modeling across the software stack used to design and model the next generation of devices. HPC resources, which have typically not been exploited in this area, are seen to be a critical enabling technology. (ENS)</p> |
| CEA | <p>Computational Electromagnetics and Acoustics</p> <ol style="list-style-type: none"> 1. TC-CEA1 – For electrically or acoustically large problems (with computational domain dimensions spanning over hundreds or more wavelengths), large-scale simulation in computational electromagnetics (CEM) and computational acoustics (CA) will require parallel methods and scalable fast algorithms. The challenge is to bring these computational technologies, such as domain decomposition, fast multipole method, matrix compression and fast solvers, which can be in research stages, to DoD production codes. (CEA) 2. TC-CEA2 – High-fidelity, full-wave antenna simulation software that enables in-situ performance characterization and rapid virtual prototyping of antennas is of high importance to the DoD design engineering and acquisition community. These problems can involve multi-scale electromagnetic simulation over electrically large computational domain, which makes HPC indispensable and will also require the incorporation of new computational technologies into DoD CEM codes. (CEA) 3. TC-CEA3/CCTA - Advancements in new computer architecture require computational electromagnetics and acoustics to look beyond the traditional computing paradigm to address the question of how CEM and CA specific techniques can be best mapped onto these architectures. The challenge is to investigate the best methodologies to implement established numerical techniques, such as finite elements, method of moments and finite element-boundary integral techniques for CEM and CA to achieve acceleration on new HPC architectures, such as GPGPU. (CEA, Cross-CTA) 4. TC-CEA4 – There is a need for an integrated design and analysis environment in computational electromagnetics (for example, in antenna and microwave hardware design). Automated design optimization has the potential to reduce design cycle time and achieve better designs through expanded search in the design parameter space. This challenge will involve the integration and automation of various software components within the HPC simulation process, including optimization, CAD/mesh generation, CEM solution and post-processing into a seamless environment for the design engineers.(CEA) 5. TC-CEA5 – Time-domain solution of linear and non-linear problems have many applications in electromagnetics and acoustics (for example, transient response, wave propagation in non-linear dispersive media etc.). Development of general purpose codes employing methods such as the finite-element time-domain and finite-difference time-domain for HPC systems will complement the capabilities in frequency domain and enable users to tackle problems where time-domain solutions are necessary.(CEA) |
| CCM | <p>Computational Chemistry, Biology, and Materials Science</p> <ol style="list-style-type: none"> 1. TC-CCM1 – Multi-scale modeling of applications in chemistry, biology and materials science. – Multi-scale modeling in support of RD&E |

activities is critical in the design of next-generation materials required for future combat systems. There is considerable effort underway to develop metallic, ceramic, polymeric, and composite materials for lightweight armor. Modeling is expected to help understand the properties of these and other important types of materials under extreme conditions and under high strain rate. Multi-scale and multi-disciplinary efforts are increasing in the area of electronic materials, which includes photonic devices, meta materials, batteries, and photovoltaic devices. Here, complex heterogeneous nano- and higher- scale environments coupled with electro-magnetic fields provide a challenge to computational methods. Construction of high-resolution, high-fidelity computer models enables a quantitative connection between the macroscopic properties of materials and the behavior of materials at the nanometer scales or micrometer scale. CCM usually takes a bottom-up approach using small-scale simulations from which homogenization often leads to development or improvement of constitutive equations at the meso/macro scale. It is challenging for CCM atomistic and coarse grain methods and data to work with the methods at the scales in other disciplines such as CSM and CFD. Furthermore, it is a challenge to identify appropriate methods for a given application or problem and develop or identify new multi-scale tools, techniques, and applications that can provide continuity between computational applications designed to operate at disparate spatial and temporal scales. (CCM, Cross-CTA)

2. **TC-CCM2 – Evaluation, implementation, and technology transfer of emerging technologies to scalable chemistry, materials science, and biology applications.** There is a persistent demand for performing larger simulations of CCM materials more accurately at all scales. Examples include mixed biological nanostructured materials used in chemical sensing and photovoltaic devices and composites of ceramics and nanostructured materials used in armor and aircraft parts. Modeling and simulation of chemistry, materials science, and biology applications benefit tremendously from software performance enhancements and especially from advances in the underlying algorithms to compute material properties more efficiently. A significant challenge in improving performance and scalability is identifying emerging algorithms and related technologies that can be adopted and then transferring the technology to the chemistry, biology, and materials science software packages that are readily used on the HPC platforms. Current trends include taking advantage of GPUs and combining non-uniform memory access shared-memory multi-core parallelism with distributed memory node-based parallelism. (CCM, Cross-CTA)
3. **TC-CCM3 – Increasing accuracy and applicability of forces.** Calculating many properties of interest in DoD materials requires a dynamical simulation, which in turn requires the evaluation of forces on the atoms of the system. A common challenge is determining whether the state-of-the-art force fields, density functionals, or other models are suitable for or transferable to the problem of interest. Advances in model potentials or functionals continue to evolve at a steady pace, but the required accuracy for a given problem often remains elusive. We can either transfer existing technology or develop it in the DoD labs. Once implemented in DoD software, significant resources are spent in tuning, evaluating, and testing the model parameters for transferability or accuracy for a given system.

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| | <p>Challenges include identifying the appropriate theories that will be used for the model-fitting functions, and developing tools to enable rapid generation of high-quality model parameters and enable the understanding of the properties of the models, for example using families of solutions provided by multi objective optimization (CCM)</p> <p>4. TC-CCM4 – Advanced data analysis and scientific visualization tools. Increasing computational power has led to the simulation of more complex problems with higher fidelity. As a result, the volume of data generated from these problems has increased by orders of magnitude. This creates data management challenges both in processing and visualizing data at this scale. Another problem is the need to manage large and diverse data sets of accurate <i>ab initio</i> or experimental data for validation and parameterization of other methods. Furthermore, the CCM community needs tools to assist with productive and efficient workflow such as automated input preparation, data processing and analysis tools. High-throughput materials discovery, such as in the materials genome project, is expected to reduce the time for development of materials and reduce the total cost. It requires new data management and analysis tools and new applications for automated work flow.(CCM, Cross-CTA)</p> |
| CFD | <p>Computational Fluid Dynamics</p> <p>1. TC-CFD1 – Productivity enhancing tools for increased throughput. Using CFD tools for design performance predictions and analysis within current timeline requirements is a challenging task. A large number of simulations is required for a design parametric study, and simply managing and monitoring the run matrix can be challenging. Significant progress has been achieved over the past few years and the focus is now on higher end high fidelity simulations with flight characteristics. Productivity bottlenecks include streamlining the single run workflow; and executing, managing and analyzing multiple simulations spanning the space of interest. For a single simulation, the user must deal with deficiencies in geometry models, mesh generation, mesh quality issues, uncertainty quantification, and results analysis. There is a need to quantify <i>a priori</i> the uncertainty in the simulation (error estimates), determine convergence criteria, and if necessary, reduce the error by implementing adaptive grid or solution technology. The traditional approaches such as grid convergence index (GCI) and time convergence index (TCI) are computationally expensive and time consuming, and they are not adequate for quantifying the error in unsteady flow computations. This necessitates the development of new approaches based on single solution error estimates. Also, the large distributed nature of the DSRC resources often requires monitoring and manual intervention for restart/recovery in the event of premature job termination. The optimum resource distribution for maximum job throughput is also challenging. These issues create critical barriers in view of throughput, efficiency, and economy of using CFD tools. This is especially true when sensitivity studies require a large number of CFD runs. (CFD, Cross-CTA)</p> <p>2. TC-CFD2 – Higher fidelity requirements and increasing system complexity. The success of DoD researchers in providing timely high quality simulations for fluid dynamic performance predictions for</p> |

configurations of moderate complexity has driven an increase in demand for such simulations. It has also generated great interest in incorporating increased fidelity and additional physical models for complex fluid physics and material and structural interactions. In particular, most emerging applications are nonlinear, discontinuous, and multi-scale, and involve multiple physical disciplines and a system with interacting components. Such problems place significant demands on numerical algorithms for multi-scale/multi-physics systems and require improved techniques for monitoring convergence, error analysis and dynamic simulation and coupling processes. For example increased-fidelity models of transitional and turbulent flows including transient and dynamic processes are required. Techniques for accurately predicting physical phenomena that span the molecular/atomic to continuum scale and drive the fidelity of a simulation are also needed. Areas of promise include high-order spatial discretizations for generalized element solution approaches and moving interface techniques with quantifiable fidelity. These capabilities are required as inputs to robust multidisciplinary design and optimization processes. Given the potential of emerging computing platforms it is necessary to explore these architectures and hybrid algorithms for proving the computational throughput for providing the required data in a timely manner. An environment that provides portability and consistency across platforms suitable for high core count execution of multiple software components is required. (CFD, Cross-CTA)

- 3. TC-CFD3 – Requirements for incorporation of additional physical models.** Modeling of chemically reacting multiphase flows is very important to the DoD in simulating rocket propulsion, projectile propellants, combustor design, turbomachinery, hypersonic aerodynamics, and chem/bio hazard tracking. Turbulence modeling remains a challenge in computational fluid dynamics (CFD). Recent developments in hybrid RANS/LES methods have improved simulations for unsteady applications, but further validation is needed. The filter functions used in these hybrid models can produce steady solutions that are not physically meaningful. Likewise, the nonlinear acoustic noise generated by an open weapons bay or a cavitating propeller represents a turbulent, unsteady flow field that requires improved unsteady turbulence models, and possibly higher-order methods, in order to provide production design turn-around times. Boundary layer transition is rarely modeled in production computations and continues to be a source of error. This error can be quite significant when CFD is used to scale subscale data to full-scale conditions, for predicting performance for high-altitude turbine engines, or when predicting heat transfer for high speed flight vehicles. Another challenge is in addressing numerical algorithms associated with phenomena involving both continuum and rarefied regions. High altitude and re-entry vehicles experience the whole range from rarefied flow to continuum flow. This requires flow solvers that can switch from rarefied flow computations to continuum computations as necessary. (CFD, Cross-CTA)
- 4. TC-CFD4 – Moving body problems.** Simulating moving body problems requires methods to: a) address the motion of bodies with multiple moving components, b) calculate grids and grid metrics for flexible bodies, c)

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| | <p>couple body movement with structural dynamics codes, d) include feedback control systems, e) detect and incorporate the influence of elastic and inelastic collisions, and f) discretize a time-dependent domain efficiently. Overset grid methods are recognized as a key technology for solving problems with moving and/or deforming bodies. Overset and unstructured methods are widely used by DoD users for solving moving body problems. However, there is a need to improve the automation, efficiency, robustness, and accuracy of overset and unstructured methods, and to expand the applicability of overset technology to new CFD codes. This is especially true for unstructured and hybrid grid strategies. Coupling single-discipline analysis codes for solving multidisciplinary problems requires some form of interface treatment and data transfer between individual codes. This is especially critical in fluid/structure interactions (FSI) where the computational mesh resolution and CPU time taken to perform a simulation are disparately distinct. If the user is solving an optimal design problem, there is also the requirement for a parametric geometry model and automatic mesh generation to efficiently deal with the deformations required to generate an optimal geometry. The fact that multiple codes are used also impacts parallelization and the requirement to maintain a level of fidelity for each component discipline. Because of the complexity of multidisciplinary problems, a framework for control and management of the simulation and optimization process is essential. (CFD, Cross-CTA)</p> |
| CSM | <p>Computational Structural Mechanics</p> <ol style="list-style-type: none"> 1. <u>TC-CSM1</u>: Design of bombs and warheads requires advancements in models to examine the burning and detonation of the explosive as well as break-up and fragmentation of the case. Modern energetic material mixtures formulated to meet insensitive munition requirements exhibit non-ideal behavior that cannot be captured with traditional equation-of-state and reactive burn models. Fracture and fragmentation models have been developed that examine breakup from a statistical point of view or through a discrete representation of the fragments. These models have been applied to proof-of-principle problems; however, they are largely unavailable in DOD weapons design software. As a result, they are not having an impact on the weapons design process. Design and forensic problems concerned with IEDs, EFPs, and shaped charges are confronted with similar issues. Designing projectiles requires an examination of projectile–target interaction and behind-armor debris. Disparities in length and time scales associated with these problems require advancements in Lagrangian, Eulerian, arbitrary Lagrangian–Eulerian (ALE), and/or meshless methods. Weapons designers are also constrained by insensitive munitions requirements and require accurate, predictive models for sympathetic detonation, bullet and fragment impact, and slow and fast cookoff. Solving these problems requires multidisciplinary approaches that combine advanced numerical solution procedures with high fidelity models for solids and structures. (CSM) 2. <u>TC-CSM2</u>: Survivability analysis requires high fidelity analysis tools to examine the loading and deformation of targets by weapons. Key technologies needed to model the interaction of structures with blast waves include accurate fluid–structure interaction (FSI) algorithms as well as |

advanced Eulerian and ALE algorithms. The problem of underwater explosions is a particularly challenging FSI problem that involves interaction of a gas bubble, water, and structure, requiring advanced interface tracking and extension to long time scales. The use of meshless methods for simulation of blast–fragment–structure interaction has gained popularity in recent years and requires a well-validated approach for modeling the loading of detonation products and gases with numerical particles in a Lagrangian framework. In the case of civil structures, the prediction of progressive damage and residual load carrying capacity is a problem of increasing concern and requires the integration of high fidelity, time-accurate models for calculation of damage and failure of structural materials, as well as extension of these models to extended time scales. Analysis of ground shock from mine and IED blast and its effect on targets is another problem critical to survivability assessment that requires advanced models for geologic materials. Armor/anti-armor analysis addresses problems of penetration, perforation, and behind-armor debris generated from projectile impact with applications to light, medium, and heavy armored vehicles and airframes, and requires integration into production-level codes of advanced algorithms for fracture, failure and fragmentation. Similarly, the penetration, perforation and debris fields of geological and construction materials are also important. Finally, ballistic and blast effects on soldiers is an extremely challenging survivability problem that pushes the envelope on Lagrangian, Eulerian, and ALE algorithms, advanced material models, and interpretation of results in terms of residual utility, mobility and/or cognitive function assessment. (CSM)

3. **TC-CSM3:** A significant portion of CSM simulations are conducted using mature, legacy software developed and tested over many years. In many cases, new and advanced material models have been developed and tested independently, but have not been yet incorporated into the legacy codes. This requirement involves incorporation and testing of advanced material models in production software used by analysts and researchers in the DoD. For example, in ballistic applications, the material model must reliably predict the stress under large strain and/or high strain rate conditions, but it may not be necessary to model other types of loading, such as shock-reshock events or time periodic loading. Exotic structural and biological materials, in particular, introduce major challenges for analysts from the perspective of identifying a suitable material model. The material model must be implemented in DoD software so that it runs efficiently and can be used easily. In the case of legacy codes, the model must also be implemented in a manner that allows seamless technology transfer to the parent code developers. Finally, as part of the implementation process, the material models must be verified and validated for use in DoD applications. (CSM)
4. **TC-CSM4:** There is a growing need for probabilistic, uncertainties and statistical modeling in nearly all CSM applications, particularly experimental design. Uncertainties in input used to run a calculation will yield uncertainties in the output. Other sources for uncertainty include those associated with models or those due to limits in accuracy in the algorithm used to represent the model. Solutions must be augmented with “error bars”

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| | <p>in the same fashion as experimental results. Many continuum mechanic phenomena are statistical in nature such as material properties, especially inhomogeneous, flaw, damage, failure and crack growth...etc. For these types of problems, classical computational mechanics are simplifications or approximations of more accurate statistical ones. Including statistical modeling in simulation provides higher fidelity computational results. Developing and implementing statistical methods and tools to improve prediction is important to CSM DOD users. (CSM)</p> <p>5. TC-CSM5: Multiscale is important to CSM DOD users in general, and the top-down multiscale approach in particular. Multiscale modeling must be looked at with an eye to producing results at continuum scales, rather than starting at the smallest scale and working upwards. More focus to meso- and micro-scales. In addition to spatial multiscale, temporal multiscale techniques are also of importance. It provides a mean to accelerate simulations in general to support the needs for DOD to simulate large models and fully detailed production structures. New state of the art temporal multiscale techniques are emerging for both implicit problems and explicit problems without shock wave. Developing and implementing temporal multiscale algorithm and method are in need for various DOD applications. (CSM, Cross-CTA)</p> <p>6. TC-CSM6: There are many complex computational issues related to DOD fully detailed production structures. Assessment of new designs, life extension of newly and existing components, and evaluation of damaged components require computational analysis tools and expertise to perform. Using modeling and simulation enable DOD users to manage and develop challenging engineering systems by representing the inherent complexities at a level of fidelity consistent with state of the art technology. For high fidelity simulation and modeling, there is a need to implement the state of the art material models, damage model, fracture model, multiscale capabilities, and uncertainties. The fact that most these efforts deal with actual complex geometry adds another level of computational challenges to the problems. (CSM)</p> |
| SIP | <p>Signal/Image Processing</p> <p>1. TC-SIP1 – The inherent complexity in utilizing and programming HPC systems is the main obstacle to widespread exploitation of HPC resources and technologies in the DoD. This need is particularly acute in the SIP and related DoD communities where typical users have various disparate, widely varying needs. Mastering the complexity of traditional programming tools and HPC environments (Linux, PBS, C, MPI, etc.) is often seen as a poor investment of resources that could be applied to the primary scientific or technical domain. Many SIP users instead prefer high-productivity/high-level languages within integrated development environments, such as MATLAB and Python. This trend is driven by a new emphasis on productivity metrics capturing time-to-solution for high-end computing systems as opposed to traditional metrics (CPU-utilization, etc.). Moreover, complexity is proliferating dramatically with the emergence of new disruptive technologies such as the availability of GPGPU, hybrid, and low-power accelerator-based systems. Consequently, the persistent challenge is to simplify the programming interface for the generic SIP user. Additionally, language</p> |

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| | <p>interoperability is important since one language or interface may be used for one purpose and another language or interface for some other purpose while desiring the two (or more) to work together. It is often necessary to integrate independently developed modules within a single application or unifying tool. Furthermore, language interoperability facilitates various language transitions, e.g., from a high-level language to a lower-level one; language interoperability improves productivity, testability, and code correctness by allowing for segmented transition process. While concept development requires high productivity languages, deployable systems may need lower-level languages. As such, appropriate language translation is desired. Finally, large memory demands are increasing for many SIP and other related applications. (SIP, Cross-CTA)</p> <p>2. TC-SIP2 – Addressing high-tempo situational awareness and actionable Intelligence, Surveillance, and Reconnaissance (ISR) capabilities within mission timelines are highly important to the DoD. Such systems and capabilities—subject to size, weight, power, and performance constraints—form a critical component of future strategic and tactical technology available to the warfighter. The challenges are multifaceted: algorithm scaling, sensor-to-processing communication, real-time signal processing amidst high-volume sensor input, exploitation of the latest HPC technologies, and the ability to provide solutions that evolve in synergy with DoD ISR requirements. (SIP, Cross-CTA)</p> <p>3. TC-SIP3 – A data deluge is upon the DoD as sensors continue to proliferate commensurate with their becoming less expensive, smaller, lighter, less power-hungry, more capable, and connected to global defense networks (including the public Internet). This is in addition to the escalation of unstructured, user-generated content. Moreover, efficient processing, structure discovery, and analytics from huge data sets, including those from distributed sensors, are becoming crucial to the operational scenarios of DoD and homeland defense systems. Making sense of this data is a demanding problem; it is one of the main SIP challenges because this data deluge outpaces current trends in hardware and software technology. This creates the challenge of being able to detect, track, extract, and/or discern—perhaps in automated fashions—critical information from large data sources. (SIP, Cross-CTA)</p> |
| CWO | <p>Climate/Weather/Ocean (CWO) Modeling and Simulation</p> <p>1. TC-CWO1 – The Impact of GPGPU Architectures on Operational CWO Applications. CWO applications parallelized by MPI and OpenMP are typically characterized by limits to their scalability on current multi-processor computer systems. Emerging GPGPU technologies may permit greater scalability, and therefore, greater computational efficiency of meteorological and oceanographic models. However, the scalability of existing models on GPGPU systems is largely unknown. Furthermore, GPGPU architectures may necessitate construction of a new generation of forecast codes to exploit them fully. A limited number of such models are already under development. (CWO)</p> <p>2. TC-CWO2 – Data Archives. CWO applications are typically data intensive. Storing observational and forecast data for a variety of requirements, such as the initialization of operational forecast models, forecast verification, visualization of post-processed data, and climate change investigations, will require archival databases of increasing size. Data classification, accessibility, residency, lifecycle, and disposition must be addressed in the construction and maintenance of</p> |

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| | <p>large database systems. (CWO)</p> <p>3. TC-CWO3 - Earth Systems Modeling. The development, verification, and operationalization of multi-component forecast systems require significant effort. Coupling paradigms and technologies present challenges and directly impact the efficiency of an application. However, component coupling in the design and construction of applications is typically labor-intensive. An interactive coupling capability through the use of a Web-based science portal might present a solution to that problem. (CWO)</p> <p>4. TC-CWO4 – Decision Support Systems. Environmental (e.g., meteorological and oceanographic) uncertainty is an important consideration in much DoD mission planning and execution. This uncertainty is generally input into performance-based, risk-reward decision models in the form of probability distributions of meteorological (and oceanographic) data. These distributions can be constructed from deterministic forecasts and historical data, but probability distributions from ensemble forecasts are generally of greater value. Nevertheless, communicating information across multiple domains, sharing data between different government agencies and DoD command structures, and visualizing model output are challenges that need to be addressed.</p> |
| SAS | <p>Space & Astrophysical Sciences</p> <ol style="list-style-type: none"> 1. TC-SAS01 – The near-space environment and upper atmosphere (e.g., ionosphere) interact strongly with high-energy particle and magnetic fluxes. These interactions have serious implications for C4I (Command, Control, Communications, Computers, and Intelligence) operations, activities, and infrastructure. Solar flares and other coronal activity are the primary sources of these fluxes and a better predictive understanding of the entire sun-earth system will enhance the DoD’s ability to prepare for, predict, and respond to threats they create. Model coupling and multi-scale codes present significant challenges and directly impact computational efficiency. 2. TC-SAS02 – The development and testing of space technologies, including hypersonic vehicles operating in the near-space regime, present significant multi-disciplinary physical and engineering challenges. Development relies on full-scale system tests and computational simulations including those of the aerodynamics, propulsion, structural integrity, thermal protection, navigation, and guidance and control of high-speed vehicles in the upper atmosphere and near-space environments. 3. TC-SAS03 – The near-space environment and upper atmosphere interact strongly with high-energy particles, radiation and magnetic fluxes. These interactions have serious implications for C4I (Command, Control, Communications, Computers, and Intelligence) operations, activities, and infrastructure. Cosmic rays and solar phenomena such as flares and other coronal activity are the primary sources of these fluxes. Better modeling of the propagation of these radiations in the operational space environment and their impact on space electronics and systems designs will enhance the DoD’s ability to design for, mitigate, and respond to threats they create. 4. TC-SAS04 – The DoD is responsible for cataloging and tracking near-earth space debris, most of which emanate from dead satellites, spent rocket motors, and collisions between objects in low-earth orbit. Better models of |

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| | <p>the extreme upper atmosphere will improve the DoD’s ability to track these objects, thereby mitigating possible hazards to satellites and spacecraft in orbit, and to predict reentry trajectories. Furthermore, ensemble and other probabilistic methods can be applied to estimate risk and probability related to space situational awareness.</p> <p>5. TC-SAS05 – A main challenge and objective is to effectively exploit high performance computing, by integrating the new space and astrophysical sciences observational data, results from space-relevant laboratory experimental programs, and advanced simulation capabilities, to generate improved predictive models of the space and astrophysical environments, and to tie together space systems performance with the complex operational environment.</p> |
| EQM | <p>Environmental Quality Modeling and Simulation.</p> <ol style="list-style-type: none"> 1. TC-EQM 1 – ADH is the flagship groundwater/surface water flow and transport simulator within the DoD (also has military applications). Improvements to ADH to accurately model complex physics and interactions are an immediate need within EQM, and have been identified as the top priority within EQM. This work requires advances in mathematical models, testing of various discretizations and linear solvers, and model coupling. (EQM, Cross-CTA) 2. TC-EQM 2 – Recent extensions of the USACE hydraulic suites from 2d to 3d required 3d visualization of both finite element and particle tracking data. 3. TC-EQM 3 – Recently, large efforts have been made to simulate multi-physics applications, resulting in the need for coupling interfaces that are portable and straightforward. 4. TC-EQM 4 – USACE requires assistance to accelerate existing code into production. This includes the use of the model to assess risk in coastal environments, contaminant propagation, etc. |
| FMS | <p>Force Modeling Systems</p> <ol style="list-style-type: none"> 1. TC-FMS1 – The proper modelling of evolving force structures and operational deployments calls for innovations in correct representation of behaviors and social networks from unfamiliar cultures and organizations using unconventional tactics. The challenge for the HPC community is to provide an environment that can support deep exploration of behavior patterns through statistical analysis of large amounts of data created through hundreds or thousands of runs of a stochastic model. HPCs also allow for exploration into computationally expensive learning techniques, such as reinforced learning methods, which were previously seen as too costly computationally, but show promise for enhancing machine learning to support commander decisions on the battlefield. Data farming, data mining, and agent-based models are a few of the key techniques in addressing this challenge. (FMS) 2. TC-FMS2 – The user community for FMS comes from a variety of venues including experimentation, analysis, and test and evaluation of current and future weapon systems. The force modeling aspect is just one component in |

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| | <p>a larger effort to perform research or test new systems. Using HPC requires the ability to work interactively with other supporting systems such as operational command and control (C2) equipment or other simulations that are not hosted on the HPC. This distributed computational environment allows the exploration of concepts in live course of action (COA) analysis and deterrence modelling. (FMS, ENS, IMT, Cross-CTA)</p> <ol style="list-style-type: none"> 3. TC-FMS3 – Mission rehearsal was hailed as a key component of success in the defeat of Osama Bin Laden. The need for rapid deployment of military personnel requires the ability to quickly create highly detailed scenarios for synthetic and live mission rehearsal and decision support. The current process can require months to develop correlated, detailed databases to support embedded live, virtual, and constructive training environments. Accelerated database generation of detailed terrain and electromagnetic effects is key to allowing responsive and timely mission rehearsal. (FMS) 4. TC-FMS4 – FMS users desire to represent simulation environments at a high level of fidelity, and they are exploring ways to include higher fidelity physics models of battlespace phenomena interacting with forces models to create a more realistic environment. In addition, the availability of additional “cloud-like” computational resources allows for representation of higher numbers of high- and medium-fidelity objects, allowing for realistic simulation of brigade level numbers or higher. (FMS) |
| IMT | <p>Integrated Modeling and Test Environments</p> <ol style="list-style-type: none"> 1. TC-IMT1 - Development of technologies that utilize the recent advances in GPGPU computing and other software tools for real-time-computing combined with Hardware-in-the-loop. 2. TC-IMT2 - Porting legacy code used for data intensive computing to HPC systems, developing software for mining of structured and unstructured data sets and real time data analysis. 3. TC-IMT3 / CCTA - Support for porting, debugging and optimizing physics based HPC applications used by T&E community and addressing special needs in coordination with other CTAs. |
| ACE | <p>Advanced Computational Environments</p> <ol style="list-style-type: none"> 1. TC-ACE2 – Architecture changes in processor technology, memory, and interconnects will continue to drive change within HPC applications. Increased parallelism with non-traditional instruction sets and performance characteristics will continue to force changes in computational methodologies needed to achieve highest levels of performance. (ACE, Cross-CTA) 2. TC-ACE2 – Although MPI has been the de facto standard for many years in HPC, some DoD users are encountering challenges that either do not map well to MPI semantics or do not have the time or knowledge to develop full applications themselves. Additional programming models and languages have the potential to bring high performance computing resources to a new set of DoD users and challenges. Other models are also of interest to users, including SHMEM, Unified Parallel C (UPC) and Co-Array Fortran (CAF). Further, many engineers are now more familiar with tools such as Matlab |

than traditional Fortran programming. (ACE, Cross-CTA)

3. **TC-ACE3/CCTA** – Increasing computational power has led to the simulation of more complex problems with higher fidelity. As a result, in many cases the data generated from these problems has increased by orders of magnitude. This creates data management challenges both in processing and visualizing data at this scale. (ACE, Cross-CTA)
4. **TC-ACE4/CCTA** – As HPC is used to solve a variety of classes of problems, workflow management and operations is a key concern. This includes data movement and analysis, non-batch processing, web-based access, and other methods of HPC access. (ACE, Cross-CTA)