DEFENSE & TECHNOLOGY PAPER 95

Report of an Army Workshop on Convergence Forecasting:
Mechanochemical Transduction

Douglas Kiserow, David Stepp, Stephen Lee, and Peter Reynolds
Edited by John W. Lyons and Richard Chait

CENTER FOR TECHNOLOGY AND NATIONAL SECURITY POLICY
NATIONAL DEFENSE UNIVERSITY

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Sponsored by the Army Research Office
Held at Noblis, Inc., Falls Church, Virginia
January 11–12, 2012

Center for Technology and National Security Policy
National Defense University

July 2012

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Acknowledgements

We thank Drs. Marilyn Freeman, David Skatrud, and Linton Wells for their support for this work.

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EXECUTIVE SUMMARY

While the rapid pace of science and technology (S&T) in the modern world is enabling new capabilities for the Army, the globalization of information, research, and economies poses new challenges for the Department of Defense (DoD) to stay at the cutting edge of S&T research and avoid technological surprise. Previous approaches to forecasting S&T abilities of future allies and adversaries, and to predicting corresponding changes required for Army strategy have had limited success. A method for more accurately predicting the emergence of future scientific discoveries and applications would be instrumental for improving the effectiveness of DoD S&T programs.

Recent studies have suggested a more successful forecasting approach: Identify potential confluences or convergences of individual science and engineering fields and then project how those convergences may lead to new capabilities. One recently emerged convergence is between the fields of chemistry and materials science. This revolutionary new field, called mechanochemical transduction, focuses on understanding and harnessing the fundamental processes through which mechanical stress can lead to a pre-designed chemical reaction.

In January 2012, the Army Research Office (ARO) sponsored the Mechanochemical Transduction Convergence Workshop as a test case for identifying convergences of disciplines and their potential impact on science and the Army. A diverse group of academic and government scientists were invited to participate in the workshop. The academic researchers were renowned subject matter experts representing a wide range of disciplines, including chemical engineering, organic chemistry, physical organic chemistry, molecular biochemistry, materials engineering, multi-scale theory, metallurgy, and physics. The chief objective of the workshop was to identify the most promising research opportunities and interdisciplinary convergences that could lead the field of mechanochemical transduction in new directions with unexpected outcomes that would be relevant to future Army needs.

I. SCIENCE AND TECHNOLOGY FORECASTING APPROACHES

A crucial role of Department of Defense (DoD) science and technology (S&T) programs is to avoid technological surprise resulting from the exponential increase in the pace of discovery and change in worldwide S&T. In addition, the nature of military threats also changes over time, resulting in changes in the capabilities required of units, vehicles, and the individual warfighter.

Since World War II, the Departments of the Army, Navy, and Air Force have sponsored several studies to predict future S&T developments to avoid technological surprise. For example, a 1947 study chartered by the Army Air Force[1] predicted a broad range of developments in aeronautics and air power and became a model for similar forecasting studies. In addition, the National Research Council (NRC) of the National Academies issues S&T projections for certain disciplines each decade and has a history of publishing S&T studies for various DoD agencies. The most recent DoD S&T forecasting studies were performed in the 1990s for the Army, Navy, and Air Force

Unfortunately, retrospective analyses of the most recent Army forecasting study have revealed significant limitations of these predictive approaches in effectively guiding research and strategy for the future Army, as is discussed further in the following section. Given that changes in the S&T landscape can lead to new capabilities *and* new requirements for the warfighter, a method to more accurately predict the emergence of future scientific discoveries and applications is needed to improve the effectiveness of DoD S&T programs. This section explores a landmark Army forecasting study, and discusses several subsequent reviews that evaluated various approaches to S&T forecasting. Recognizing the limitations and potential advantages of various forecasting methods reveals the rationale for the forecasting approach used in the Mechanochemical Transduction Convergence Workshop. In the chapters that follow, we look at an Army forecast (STAR21) from the early 1990s—what it covered and how well it predicted events from a review conducted some 15 years later. Next we introduce the approach we call convergence forecasting. A workshop to study the efficacy of the approach has been designed at the Army Research Office using the topic mechanochemical transduction as the principle focus, and the details of the workshop are provided. The report ends with a summary and conclusions

II. LANDMARK ARMY STUDY OF S&T FORECASTING—STAR21

The most recent S&T forecasting study for the Army, *STAR 21—Strategy Technologies for the Army of the Twenty-First Century*, was completed by NRC and published in 1992.[2] Similar studies were also performed for the Air Force[3] and the Navy.[4] Based on their predictions of the future S&T landscape, these studies have been used to guide certain aspects of DoD-wide

[1] Theodore von Karman, *Toward New Horizons* (Washington, D.C.: United States Army Air Force, 1945).

[2] Board on Army Science and Technology, Commission on Engineering and Technical Systems, National Research Council, *STAR 21—Strategic Technologies for the Army of the Twenty-First Century* (Washington, D.C.: National Academy Press, 1992).

[3] Air Force Scientific Advisory Board, *New World Vistas, Air and Space Power for the 21st Century* (Washington, D.C.: Department of the Air Force, 1995).

[4] Naval Studies Board, National Research Council, *Technology for the United States Navy and Marine Corps, 2000–2035* (Washington, D.C.: National Academy Press, 1997).

research. The STAR 21 study aimed to predict the future S&T environment and the corresponding impact on Army capabilities and strategy at least 30 years into the future (i.e., through 2020). The study had three specific objectives:

1. Identify the advanced technologies most likely to be important to ground warfare in the next century
2. Suggest strategies for developing the full potential of these technologies
3. Project implications for force structure and strategy of the technology changes

To reach these goals, NRC organized panels focused on various aspects of these three main objectives. These committees were diverse and composed of scientists, physicians, and other subject matter experts (SME) from academia, industry, and government. To accomplish the first objective, the study assessed state-of-the-art S&T of that period, and forecasted the technology that was likely to be available within 10 to 15 years and relevant to the Army, which could potentially be included in Army systems by 2020. The predicted technologies were divided into eight technology groups based on the most likely Army application; examples of these groups include electronics and sensors, biotechnology and biochemistry, and advanced materials. In addition, a long-term forecast of research identified 11 major technological trends expected in the next 30 years that would cut across the traditional boundaries of scientific disciplines, such as the information explosion, chemical synthesis by design, and the use of hybrid materials. Regarding the second objective, the study considered the technologies predicted in the first objective and then identified five Army-relevant systems through which the Army could most effectively integrate the future technologies to meet the principal mission areas, such as integrated support for the Solider, combat power and mobility, and winning the information war. Lastly, the study identified the potential implications of the future S&T environment to Army force structure and strategy.

Many of the conclusions of the study considered the state of the Army and its observable capabilities at the conclusion of the 1991 Gulf War. A key recommendation of the study was that the Army should maintain its current level of support for research and advanced technology (i.e., 6.1-, 6.2-, and 6.3a-funded research), despite an anticipated reduction in overall research funding available for acquisition.

The STAR 21 study informed Army leadership of the future importance of particular technologies and increased the awareness of the impact of S&T on the Army's future capabilities at both the Army and DoD levels, as well as to congressional staff. The study also provided input to the Army's principal S&T planning document: the Army Science and Technology Master Plan. Unfortunately, the accuracy of the STAR 21 predictions and the validity of its forecasting approach remained unknown until years later as discussed below.

STAR 21 IN RETROSPECT

Although it was well recognized that accurately forecasting S&T discoveries and developments 30 years in the future is very difficult, the accuracy of the STAR 21 study's predictions can only be assessed in retrospect. Given that a forecasting study's prediction of the future S&T landscape is foundational to recommendations for future Army force structure and strategy changes, assessing the predictive accuracy of the STAR 21 study could be used to improve the approaches used in subsequent forecasting studies.

The Center for Technology and National Security Policy (CTNSP) completed a review of the STAR 21 report in 2008.[5] This review assessed the accuracy of the study's predictions and revealed potential limitations in the underlying approach used by STAR 21 to forecast the future of S&T. The CTNSP assessment indicated that after 15 years, about 25 percent of the predictions were on target, while the remaining predictions were incorrect, overly optimistic, or too conservative. In other words, approximately 75 percent of the predictions were inaccurate after only 15 years. In addition, several pivotal S&T capabilities that emerged during that 15-year period were not predicted in the STAR 21 report, such as the impact of the Internet and the World Wide Web, the proliferation of personal computational devices, and the spread of wireless technology. (Complete details of the analysis of the STAR21 review are found in reference 5.)

The CTNSP review of the STAR 21 study noted that evolutionary changes in S&T are easier to predict, while revolutionary developments are more difficult. Interestingly, the assessment also found that in general, STAR 21, as in similar studies by the Air Force and Navy, did not consider the future capabilities of individual systems with reference to the underlying sciences. The separation of future capabilities from the underlying S&T forecasts may have contributed to some of the study's inaccurate and missed predictions.

Given the rapid pace of technological change and the observed limitations of the STAR 21 study, the CTNSP review concluded that new approaches are needed to effectively forecast the future of S&T and the corresponding impact on the Army. The review also provided nine recommendations for the design and approach of future forecasting studies, such as (i) allow no more than 10 years between forecasting studies, (ii) forecasting studies should not cover all areas of technical interest at once, and (iii), the basic and applied aspects of an S&T field should be studied and reported together.

A NEW STRATEGY FOR S&T FORECASTING

In 2009 and 2010, the CTNSP issued two key papers that documented numerous cases where well-recognized capabilities and/or new scientific fields emerged because two or more scientific disciplines converged.[6-7] In this context, convergence is defined as the multidisciplinary synergy of two or more research disciplines to create a new research area, capability, and/or technology that would probably not have emerged through exclusive study within a single area.

A few examples of convergence are listed below.

- Basic research in electromagnetic radiation and the development of microwave generators, transmitters, and power supplies converged to result in the advent of radar in 1936.[8]

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5 John Lyons, Richard Chait, and Jordan Willcox, *An Assessment of the Science and Technology Predictions in the Army's STAR21 Report,* Defense & Technology Paper 50 (Washington, D.C.: Center for Technology and National Security Policy, July 2008).

6 John Lyons, Richard Chait, and James Valdes, *Forecasting Science and Technology for the Department of Defense,* (Center for Technology and National Security Policy, November 2009).

7 John Lyons, Richard Chait, and Simone Erchov, Editors, *Improving the Army's Next Effort in Technology Forecasting*, (Center for Technology and National Security Policy, September 2010).

8 Timothy Coffey, Jill Dahlburg, and Elihu Zimet, *The S&T Innovation Conundrum,* Defense & Technology Paper 17, (Washington, D.C.: Center for Technology and National Security Policy, August 2005).

- Genomics and information technology converged to form the new field of systems biology, which opened the door to individualized medical treatments and rational drug design based on differences at the molecular level rather than treatments based on group norms and averages.
- Research in atomic physics leading to improved atomic clocks, computer sciences, communications technology, electronics, and space vehicle technology converged to enable the Global Positioning System.
- Research in optical physics and materials science converged to enable night-vision capabilities.

When one considers these and other examples[9] of revolutionary capabilities that radically changed the battlefield over the past 50 years, it becomes evident that these capabilities all emerged from scientific advances across multiple research areas.

The CTNSP reports concluded that since convergences have historically led to revolutionary S&T capabilities, creating "roadmaps" that outline potential convergences could provide a type of targeted forecasting that could predict revolutionary scientific discoveries, applications, and their corresponding impact on the Army. More specifically, the report recommended that technology forecasting should begin by (i) listing the outcomes and associated capabilities desired by the Army at a future time point, and then (ii) identifying confluences or convergences of individual sciences and technologies that would enable the realization of such capabilities. In addition, these papers concluded that it is possible to create an atmosphere within the Army's research planning and investment activities that would enhance the probability that such convergences would occur, and would shape multidisciplinary research such that the convergences occur in directions most likely to benefit the Army.

Interestingly, the 2010 CTNSP paper examined the clustering of research in chemical sciences and materials science that appear to be converging and giving rise to a new field: mechanochemical transduction. Mechanochemical transduction was then identified as a suitable case study to continue exploring the potential of these new S&T forecasting approaches, as is discussed further in Section III.

III. WORKSHOP ON CONVERGENCE FORECASTING: MECHANOCHEMICAL TRANSDUCTION

As discussed in the previous section, the landmark 1992 Army S&T forecasting study, STAR 21, was found to have poor predictive accuracy due in part to certain limitations in its forecasting methods. The subsequent CTNSP reviews of the STAR 21 study concluded that new approaches are needed to effectively forecast the future of S&T for the Army.

The Army Research Office (ARO), working with the Army S&T staff, held the 2012 Mechanochemical Transduction Convergence Workshop as a pilot approach for how a convergence forecasting study could be conducted. This workshop brought together researchers and government staff to predict how future convergences in mechanochemical transduction could result in revolutionarily Army capabilities or could result in changes in the S&T landscape

[9] Refer to the aforementioned CTNSP articles for descriptions of other examples of convergence.

that would change Army force requirements. This workshop incorporated and tested the efficacy of many of the recommendations outlined by CTNSP in references 6 and 7 for use in future forecasting studies.

OVERVIEW OF MECHANOCHEMICAL TRANSDUCTION

Mechanochemical transduction is an emerging field at the intersection of chemistry and materials science that focuses on understanding and harnessing the fundamental processes through which mechanical stress can lead to chemical reaction. This research area involves the design and creation of materials at the molecular level such that when sufficient mechanical stress is exerted on the material in the proper orientation, the material responds at the molecular level with a pre-determined chemical reaction that changes the structure and properties of the material. The long-term goals of this research are to design mechano-responsive molecules called mechanophores, and incorporate these molecules into materials, such as composites and coatings, to confer mechano-responsive properties. When subjected to mechanical force, the mechanophores within the bulk material will generate chemical changes, which if properly designed, result in beneficial macroscopic changes such as self-sensing or self-healing.

Progress in this research area is contingent on people from a number of disciplines (e.g., chemists, materials scientists, and engineers) working cooperatively to design and synthesize mechanophores, incorporate them into material systems, and evaluate the mechanochemical response. Although there are only a few coordinated efforts of this type, ARO has taken a lead in this area since 2006 by supporting multidisciplinary programs to drive this research convergence into the future.

Given that mechanochemical transduction is a new field at the forefront of a convergence between chemistry and materials science, this topic was identified as a suitable case study to explore new approaches for forecasting future S&T and to explore new methods for driving this research in directions likely to result in new Army-relevant capabilities.

WORKSHOP OBJECTIVES AND APPROACH

The goal of the workshop was to identify the most promising research opportunities and interdisciplinary convergences likely to extend and mature the field of mechanochemical transduction in ways relevant to Army needs. More specifically, the overall objectives of the Workshop were to:

1. Assess the current state of research in mechanochemical transduction across disciplines
2. Identify promising, long-range, S&T capabilities that may emerge and are relevant to Army capabilities
3. Identify key barriers to success
4. Identify convergence milestones necessary to achieve the long-range outcomes

To meet these overall objectives, a diverse group of academic and government scientists were invited to participate in the workshop. Care was taken to invite academics with complementary interests and knowledge. The academic researchers who attended were SMEs across a wide range of disciplines, including chemical engineering, organic chemistry, physical organic chemistry, molecular biochemistry, materials engineering, multi-scale theory, metallurgy, and physics.

ARO organized and managed the workshop, along with Professor Josef Michl, University of Colorado, Boulder, who also served as a technical advisor. In addition, three government SMEs were invited to help provide the Army perspective on current Army S&T technical challenges. Three additional government staff representing the Deputy Assistant Secretary of the Army for Research and Technology (DASA[R&T]) and the National Defense University (NDU) also attended to observe how the workshop was conducted. A complete list of attendees is provided in Appendix A.

To accomplish the workshop's objectives of exploring convergence in mechanochemical transduction and determining how potential advances could lead to new capabilities for the Army, the workshop organizers designed a dynamic approach involving small-group "breakout sessions" and no formal presentations. (The agenda for the workshop is provided in Appendix B.)The execution of the meeting evolved in real time as the meeting progressed. To the knowledge of the organizers and participants, this approach had never been used before in a workshop. The goals and results of these sessions are presented in the following section.

DETAILS OF THE WORKSHOP

As introduced in the previous section, this workshop used a non-traditional format designed to achieve the overall objectives. Rather than using a traditional seminar format with PowerPoint presentations, which often limits communication to one dimension (i.e., presenter to audience), the organizers designed an interactive approach whereby the participants interacted in synergistic, cross-disciplinary, small group discussions.

As illustrated in Figure 1, the workshop included three breakout sessions scheduled across 2 days, with participants organized into groups and tasked to identify research areas with the greatest potential to converge at a new breakthrough in mechanochemical transduction, and how to shape these convergences to meet future needs of the Army. The dynamic nature of the workshop enabled the organizers to assess the results of each breakout session and use feedback from participants and the breakout groups' reports to determine the optimal objectives and format for the subsequent session.

The workshop began with the organizers introducing the academic participants. The organizers discussed how each researcher's interests and experience were likely to contribute to the goals of the workshop, which ensured that attendees were aware of the rationale for each participant's invitation to the workshop. After these introductions, the academic participants briefly summarized their research interests, and then the government attendees presented their research interests and noted their areas of expertise regarding Army needs and capabilities.

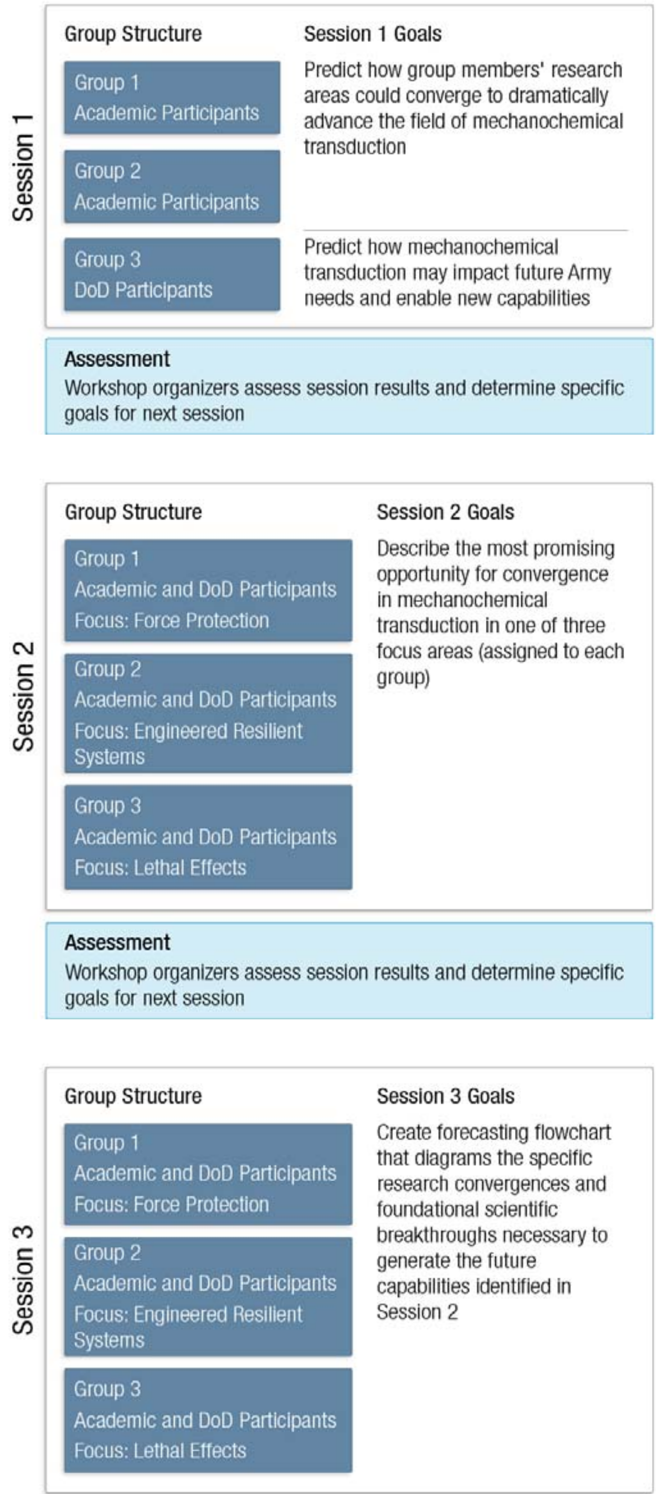

Figure 1. Mechanochemical Transduction Convergence Workshop Format

The workshop did not consist of traditional slide presentations in seminar format; rather, the focus was on interactive, dynamic, cross-disciplinary small group discussions.

IV. WORKSHOP RESULTS

SESSION 1

The first breakout session consisted of three groups, composed of either academic or government participants. The academic participants were grouped separately from government participants to ensure that the academic groups initially focused on the scientific aspects of convergence. With guidance from the workshop organizers, the academic participants were allowed to self-select the membership of their breakout groups (Group 1 and Group 2) based on other researchers with whom they thought their research interests were most likely to form convergences. The government attendees formed a separate group (Group 3).

The objectives of the academic and government groups differed (refer to Figure 1). The two academic groups were tasked to identify and forecast which of their research interests could potentially intersect in a convergence with complementary research from the other academics. The objective of Group 3, the group composed of government attendees, was to identify the near-, mid-, and long-term Army mission requirements that could be met with potential capabilities that could emerge from continued research in mechanochemical transduction.

<u>Group 1</u> identified potential convergences and new capabilities focused on the concept of remodeling, in which a material could “sense” mechanical damage and induce chemical changes where repair or realignment is needed. The following key concepts and future capabilities were forecasted by this group:

- Smart failure: failure at predetermined locations; having things break in such a way as to enable repair or enhance strength
- Based on the concept that paper is a remarkably strong material, use it to create a material that transduces orthogonal force into in-plane force
- Transformation-induced plasticity, based on concepts in metallic systems
- Use structured fluids to deliver forces locally to molecules
- Consider liquid crystals for amplification: their behavior is highly nonlinear
- “Mechanosetting” materials
- Functionalized fibers where a phonon along a fiber induces a process
- Chemical capacitors to ensure self-healing materials have high potential energy
- Mechanochemical changes do not have to happen all at once; they could be designed to occur in stages

The conclusions of Breakout Session 1, Group 1 regarding the major factors governing remodeling are summarized in Figure 2. The group noted that to drive the realization of these future research topics and capabilities, additional research would be required to further existing progress in investigating systems of material remodeling.

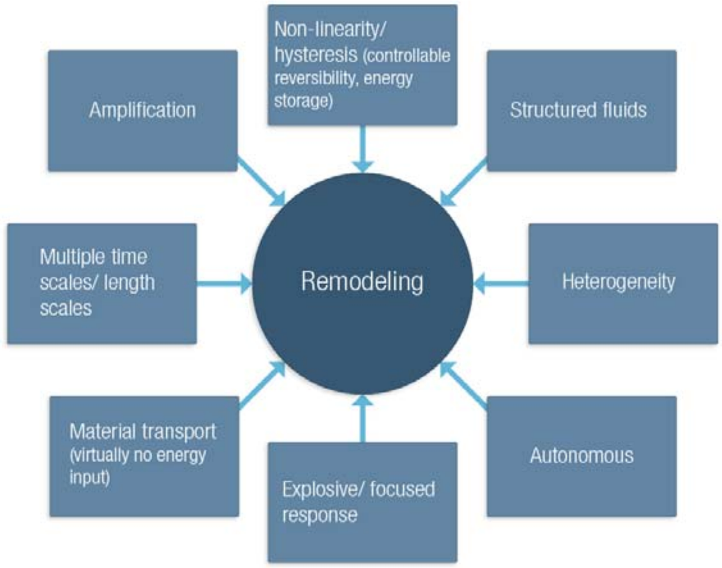

Figure 2. Results of Breakout Session 1, Group 1
The group identified several concepts that will govern future advances in remodeling capabilities.

Group 2 forecast the potential use of ultrasound as a mechanism to induce mechanochemical reactions. If ultrasound is to be used to provide the mechanical energy for subsequent chemical reactions, cavitation is required; however, it is currently difficult to identify whether cavitation is occurring at the molecular level. The group identified several potential future capabilities, focusing on the use of ultrasonics at solid-solid interfaces that may be enabled by convergences in mechanochemical transduction (see Figure 3).

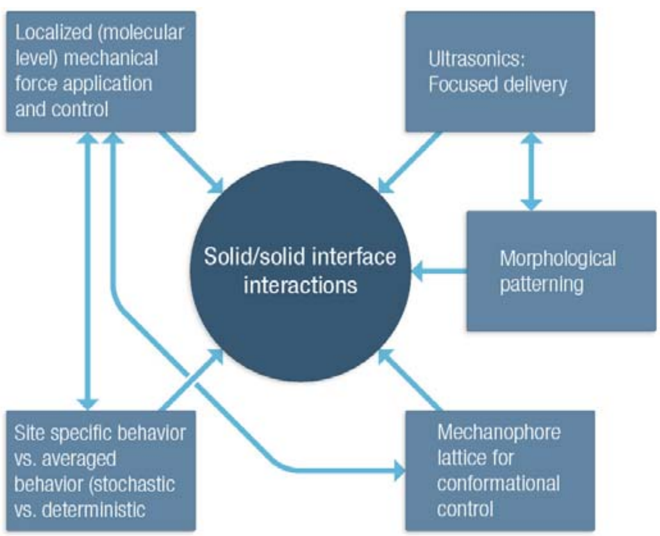

Figure 3. Potential Ultrasound-Mediated Capabilities in Mechanochemical Transduction
Group 2 of Breakout Session 1 identified these potential ultrasonic-based mechanochemical transduction capabilities.

In addition, the group identified various factors that will limit the use of ultrasound-mediated mechanochemical transduction. They require further study to drive the emergence of these capabilities in the future (see Figure 4).

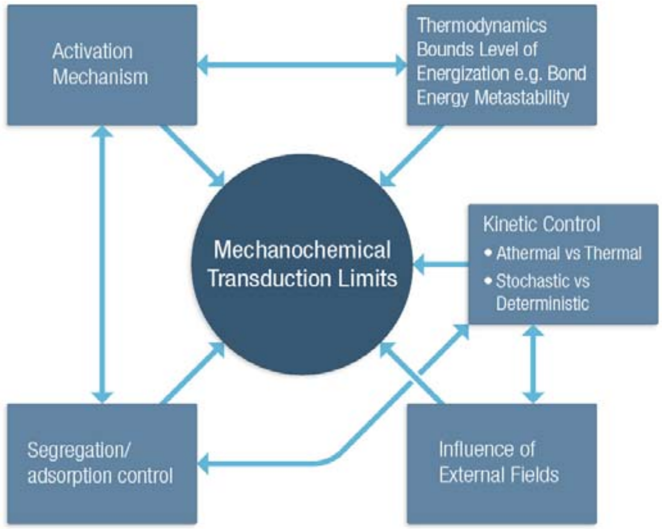

Figure 4. Factors that Limit Potential Ultrasound-Mediated Mechanochemical Transduction Capabilities

Group 2 of Breakout Session 1 identified these factors as a potential limit to the use of ultrasound-mediated mechanochemical transduction.

Group 3, composed of government participants, identified where and how potential new capabilities emerging from research in mechanochemical transduction may enable new Army capabilities and/or change Army force requirements over the next 20 to 30 years.

The group noted that compared to other physical and chemical phenomena, mechanochemical transduction is a less familiar domain, especially among the DoD user community. Therefore, in the ensuing discussions, the group struggled with whether mechanochemical transduction is a viable way to deliver the desired properties. While the group acknowledged that not all the concepts could be optimally realized through mechanochemical transduction, any concept or application that might benefit from mechanochemical transduction was considered, in recognition of the importance of avoiding technological surprise.

Ultimately, Group 3 identified following three primary topic areas of interest to the Army that could potentially be impacted by mechanochemical transduction research:

- Force protection
- Engineered resilient systems
- Lethal effects

SESSION 2

As discussed previously, the unique and dynamic nature of the workshop required the organizers to review the results of the previous session to determine the most appropriate group organization and objectives for the subsequent session.

Given that the Session 1 academic groups had successfully identified several potential scientific convergences in the area of mechanochemical transduction, and the government group had identified key areas of Army interest potentially influenced by ongoing research in mechanochemical transduction, the organizers determined that Session 2 would include three groups, each composed of academic researchers and at least one government representative. The government representatives were incorporated into these groups to provide guidance on Army needs and capabilities.

The session objectives were to identify the most promising opportunities for a substantial convergence in mechanochemical transduction that would impact aspects of the 24 Army S&T challenges.[10] Each group was given one challenge area on which to focus its discussion: force protection, engineered resilient systems, or lethal effects (refer to Figure 1).

SESSION 2

Group 1 of Session 1 identified a new penetration-resistant material as a capability that could potentially be enabled by convergences in mechanochemical transduction and would meet the Army S&T challenge area of Force Protection. As described below, the group defined how mechanochemical transduction could enable this new capability, identified the convergences required, and presented key scientific questions for future investigative research that must be addressed to enable these convergences.

- Capability: A material that absorbs shock energy and disperses shock pressure, decreasing below lethal levels, and uses energy to transform material to a form able to resist subsequent penetration of fragments
- Required convergences
  - Trauma/physiology
  - Shock physics/fluid dynamics
  - Chemical kinetics
  - Blast anatomy
  - Material design
  - Mechanics engineering
  - Non-linear dynamics
- Key scientific questions:
  - How do you stop a shock?
  - Can non-linear mesoscale structures control shocks?
  - Could material reaction be automatically reversible post-impact?

[10] The office of DASA(R&T) recently reported the 24 Army S&T Challenges of the future. A list of these challenges is available at: *https://www.alt.army.mil/portal/page/portal/oasaalt/SAAL-ZT.*

- How will lamellar structures provide interfaces for multiple responses (Initiate reactions? Disperse shocks? Absorb energy through interface delamination?)?
- What material transformations are needed to defeat fragments?

Group 2 identified a capability that could potentially be enabled by convergences in mechanochemical transduction and would meet the Army S&T challenge area of Engineered Resilient Systems. The group defined the concept of a "Molecular Foundry" as a set of methods and concepts in materials science, not yet identified, able to capitalize on harvesting the mechanical energy in materials that is currently dissipated and capturing that energy to power active sensing and regenerative capabilities. This Molecular Foundry would include a variety of beneficial features for new capabilities, but would require addressing several scientific challenges and also the convergence of multiple scientific areas.

- Features of the Molecular Foundry:
  - Design of components at the molecular scale with the ability of molecules to "talk" to components
  - Radically new level of processing to result in new material properties
  - Intelligent dynamic control anticipated during material design
  - Cost benefits
- Scientific challenges associated with realizing the Molecular Foundry:
  - Ability to exploit a wide spectrum of mechanical energy
  - Ability to operate across size scales from molecular to mesoscopic, encompassing transitions from phase transitions to chemical bonds to electron transfer
  - Ability to realize a self-aware sensing paradigm across length scales
- Realization of the Molecular Foundry demands convergence of many fields, including fluid dynamics, computer science, materials science, mechanical engineering, biochemistry, biophysics, biomimetics, synthetic chemistry, and others

As an example of the potential applications of this Foundry, the group identified mechanochemically triggered polymeric materials for manipulating mechanical force as a potential capability that could address aspects of the Army's needs in Engineered Resilient Systems. For example, this capability could enable the use of energy from a mechanical impact to stop subsequent bleeding, a body-temperature trigger to shift weight load of soldiers carrying heavy packs, and regenerative materials to store energy and provide recovery properties.

Group 3 identified new energetic materials as a capability that could be enabled by convergences in mechanochemical transduction and could meet the Army S&T challenge area of Lethal Effects. More specifically, the group identified the following capabilities as potentially relevant for addressing the Army's challenge area of Lethal Effects.

- Energetics where the rate of energy release can be better controlled
- Changing the sensitivity of energetics by controlling the defects (possibly relieving stress)
- Controlling microstructure of energetics (polymorphs, seeding crystal formation and growth)
- Pressure effects on reaction kinetics
- Delivery of same explosive force with less weight

SESSION 3

At the conclusion of the first day of the workshop (i.e., after completion of Sessions 1 and 2), the organizers compiled reports from all groups in the first two sessions and feedback from individual participants. The organizers assessed these results to determine the objectives for the final session of the workshop.

The organizers concluded that the participants found key research areas that would lead to research breakthroughs and may converge to enable future capabilities relevant to the Army; however, the groups did not identify where specific research convergences must occur to form the foundation of these capabilities. The membership of each group in Session 3 remained the same as for the previous session, and the groups were tasked to explore their previous results and create a forecasting roadmap to identify the convergences that must occur to enable the future Army capabilities previously identified in Session 2.

Group 1 of Session 3 identified four scientific breakthroughs that could be enabled by convergence of disparate scientific disciplines leading to a material with a targeted application (see Figure 5).

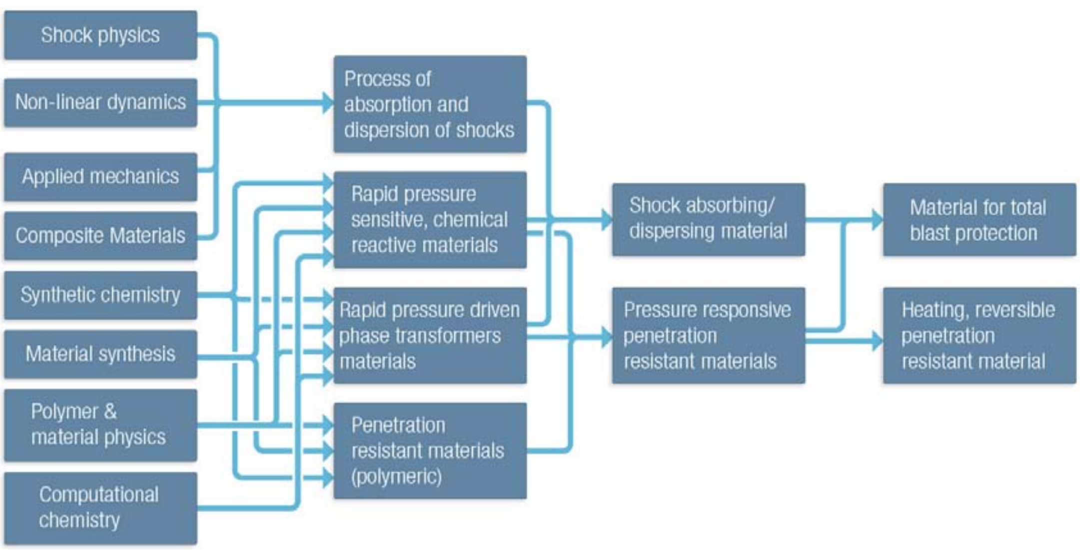

Figure 5. Forecasting New Capabilities and Required Convergences for Force Protection
Session 3, Group 1 outlined the mechanochemical transduction convergences required to enable new capabilities for addressing Army needs in Force Protection.

<u>Group 2</u> expanded the conceptual model of the Molecular Foundry to identify the areas of research and development that must converge to enable the Foundry. The group constructed a process flow diagram, as represented in Figures 6 through 8.

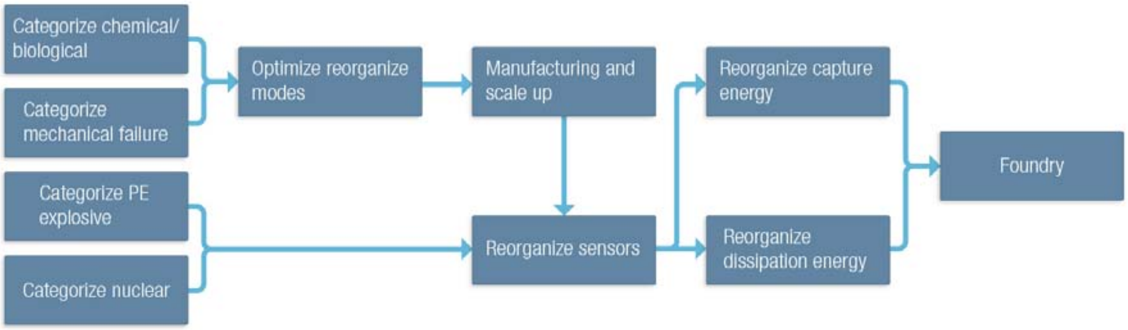

Figure 6. The Molecular Foundry

Session 3, Group 2 outlined how a conceptual Molecular Foundry of the future could leverage energy capture and dissipation to enable applications in various domains.

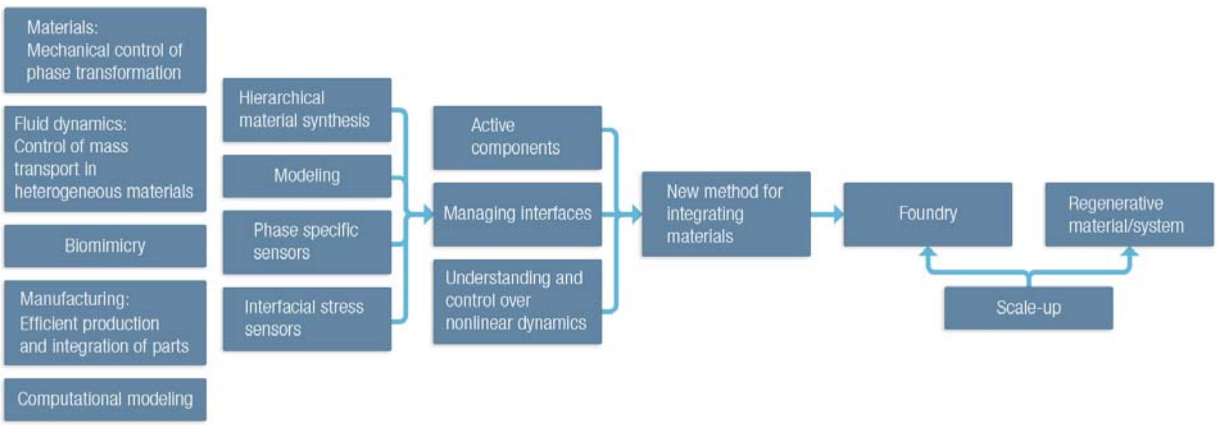

Figure 7. Forecasting Required Convergences to Enable Property Engineering

Session 3, Group 2 outlined the projected mechanochemical transduction convergences that will enable the engineering of new properties, such as interface design, and may generate new Army capabilities in Engineered Resilient Systems.

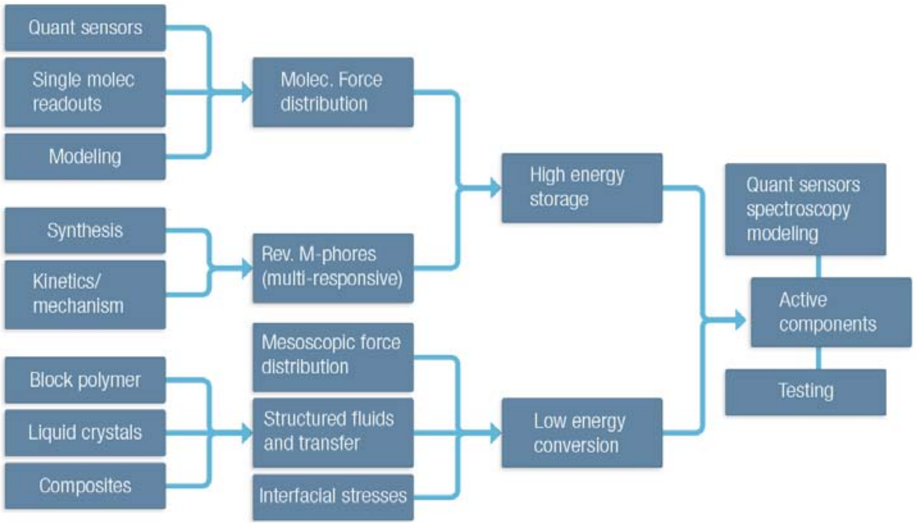

Figure 8. Forecasting New Capabilities and Required Convergences for Engineered Resilient Systems

Session 3, Group 2 outlined the active components of the high-energy storage and low-energy conversion processes that enable this new method for integrating materials using the Foundry concept.

Note that Group 3 revisited the concept of enhanced-lethality materials, considering all the possible contributing scientific fields and what convergences must result that would enable this new capability. The group generated a convergence forecasting flowchart to illustrate these concepts (see Figure 9).

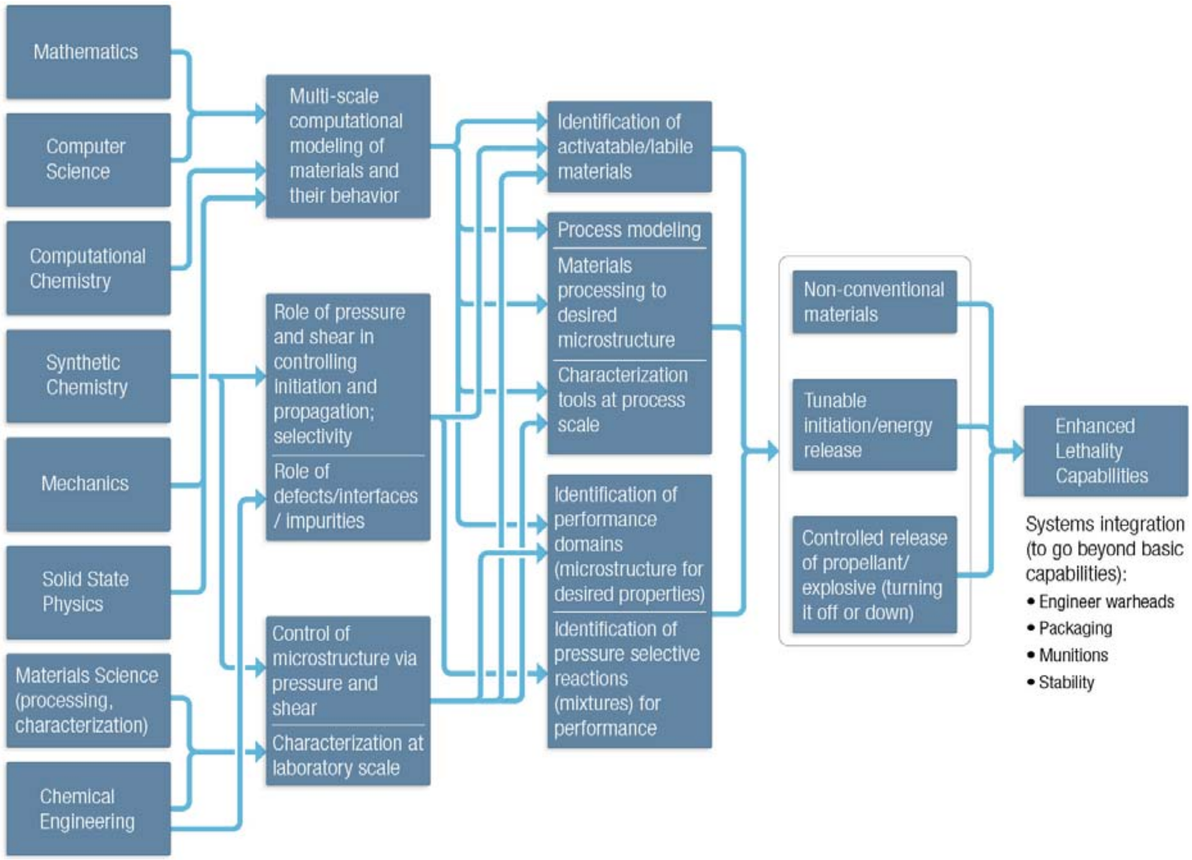

Figure 9. Forecasting New Capabilities and Required Convergences for Lethal Effects
Session 3, Group 3 outlined the underlying scientific fields that must converge and the scientific barriers that must be overcome to enable enhanced-lethality materials based on mechanochemical transduction concepts.

V. SUMMARY AND CONCLUSIONS

In January 2012, the ARO held the Mechanochemical Transduction Convergences Workshop to identify promising convergences of scientific disciplines and their impact on science and the Army. A diverse group of academic and government scientists representing chemical engineering, organic chemistry, physical organic chemistry, molecular biochemistry, materials engineering, multi-scale theory, metallurgy, and physics were assembled. The focus of the workshop was to identify the most promising research opportunities and interdisciplinary convergences that could lead the field of mechanochemical transduction in new directions with unexpected outcomes that would be relevant to future Army needs and capabilities.

In the preliminary phase of the workshop, where academic and government participants were kept in separate groups, academic discussions identified convergences surrounding the themes of remodeling (a material could “sense” mechanical damage and induce chemical changes where repair or realignment is needed) and ultrasound (as a mechanism to induce mechanochemical reactions, particularly at solid-solid interfaces). Preliminary government discussions identified relevant Army capabilities surrounding the themes of force protection, engineered resilient systems, and lethal effects.

In the final phase of the workshop, discussions integrating academic and government perspectives produced three convergence roadmaps. These convergence roadmaps outlined where and how the synergy of two or more research disciplines is likely to lead to scientific breakthroughs enabling a new research area, capability, and/or technology. The first convergence roadmap, targeting the theme of force protection, predicted a material that absorbs shock energy and disperses shock pressure (decreasing below lethal levels), and that uses energy to transform and resist subsequent penetration of fragments. The key scientific breakthroughs predicted to enable such a capability were: rapid pressure-sensitive chemically reactive materials, and rapid pressure-driven phase transforming materials. Both of these breakthroughs were predicted to result from the convergence of synthetic chemistry, materials synthesis, polymer and material physics, and computational chemistry.

The second convergence roadmap, targeting the theme of engineered resilient systems, predicted the sublimation of energy from a mechanical impact to stop subsequent bleeding and initiate wound treatment, a body-temperature trigger to shift weight load of soldiers carrying heavy packs, and regenerative materials to store energy and provide recovery properties. The key scientific breakthroughs predicted to enable such a capability were the ability to controllably capture and dissipate energy, and the ability to design and manage material interfaces. The first breakthrough was predicted to result from the convergence of quantitative sensors, single-molecule-readouts modeling, synthesis, and kinetics; the second from the convergence of hierarchical materials synthesis, modeling, phase-specific sensors, and interfacial stress sensors.

The third convergence roadmap, addressing lethal effects, predicted new energetic materials with dramatically controlled sensitivity and rate of energy release. The key scientific breakthroughs that were predicted to enable such capabilities were the identification of materials that are labile or can be activated, and of pressure-selective reactions. Both of these breakthroughs were predicted to result from the convergence of multi-scale computational modeling, synthetic chemistry, materials science, and chemical engineering.

Accurately forecasting science and technology discoveries and developments is extraordinarily challenging and difficult to assess. The accuracy of a study’s predictions can only be assessed in retrospect; however, several significant conclusions can be drawn regarding the effectiveness of the Mechanochemical Transduction Convergences Workshop. First, the dynamic approach that used small-group “breakout sessions” and no formal presentations, evolved in real time as the meeting progressed, and produced unique results. In particular, this approach focused the discussions on capabilities and scientific disciplines that had been jointly established as the most promising by the government and academic participants. This minimized external biases and enabled discussions and themes to adapt and evolve based on the interactions of the expert participants. Second, the dynamic approach with a small group of experts catalyzed the formation of a new community of government and academic researchers with a common vision for advancing the science of mechanochemical transduction and for providing new capabilities to the Army. Third, while no new specific scientific convergence was identified, the results from the three convergence roadmaps are highly consistent with the most recent opportunities identified by the ARO basic research program managers who have led the Mechanochemical Transduction Program from its inception.

In summary, this workshop was found to be an effective means for bringing the academic and government research communities together to explore how several disciplines could work together to advance a research area in new, beneficial directions that could lead to new Army capabilities. The result is that several promising research directions were identified. The convergence technique should be useful, when used with other approaches, to help design the Army's S&T portfolio.

APPENDIX A: LIST OF ATTENDEES

Professor Nicholas Abbott
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LTC Timothy Warner
U.S. Army Research Office

Ms. Ann Breckenkamp
Ms. Cathy Cotell
Mr. Rick Rhoads
Mr. David Roberts
Noblis, Inc.

APPENDIX B: WORKSHOP AGENDA

Day 1—Wednesday, January 11, 2012

Time	Agenda Item	Speakers/Leaders
0800–0830	Registration and coffee	
0830–0840	Administrative remarks	Rhoads, Stepp, Kiserow
0840–0910	Introduction to Mechanochemical Transduction and Convergence Forecasting	Stepp, Kiserow, Lee, Reynolds
0910–0930	Alignment of attendees and workshop goals (Academic attendee introductions)	Stepp, Kiserow
0930–1000	Government attendee introductions	Government attendees
1000–1030	Break	
1030–1130	Academic research area descriptions and Q&As	Academics
1130–1200	Academics list others they wish to work with to determine convergences (ARO organizers assign three groups)	Stepp, Kiserow
1200–1300	Lunch	
1300–1530	Breakout assignments and Breakout Session #1 discussions	Stepp, Kiserow
1530–1600	Break	
1600–1700	Breakout group reports	Academic Groups
1700	Day 1 Wrap up	Stepp, Kiserow

Day 2—Thursday, January 12, 2012

0830–0900	Administrative remarks. Underline focus on convergences.	Stepp, Kiserow, Reynolds
0900–1000	Approaches to Army S&T Briefing	Scharf
1000–1030	Academics list others they wish to work with to determine convergences (ARO organizers assign three groups)	Stepp, Kiserow
1030–1130	Breakout Assignments and Breakout Session #2 discussions	
1130–1200	Breakout group reports	Academic Groups
1200–1330	Working lunch Breakout assignments and Breakout Session #3 discussions (same groups as Session #2)	
1330–1400	Breakout group reports	Academic Groups
1400–1430	Break	
1430–1500	Day 2 Wrap up	Stepp, Kiserow