U.S. ARMY COMBAT CAPABILITIES DEVELOPMENT COMMAND – ARMY RESEARCH LABORATORY

High-Throughput Materials Discovery for Extreme Conditions (HTMDEC) Year 1 Kickoff Meeting
12 & 13 JULY 2022

Chris Haines, Debjoy Mallick, Scott Schoenfeld
CAM, Deputy CAM, ST-Terminal Ballistics
WMRD
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>1300</td>
<td>Welcome and Introductory Remarks</td>
</tr>
<tr>
<td>1315</td>
<td>Army Research Lab Executive Greeting</td>
</tr>
<tr>
<td>1330</td>
<td>HTMDEC OV &amp; Program “Calendar” – Haines/Mallick</td>
</tr>
<tr>
<td>1415</td>
<td>Texas A&amp;M Univ – Raymundo Arroyave (or alternate)</td>
</tr>
<tr>
<td>1430</td>
<td>Georgia Tech Univ – Surya Kalidindi (or alternate)</td>
</tr>
<tr>
<td>1445</td>
<td>Univ California San Diego – Kenneth Vecchio</td>
</tr>
<tr>
<td>1500</td>
<td>Break</td>
</tr>
<tr>
<td>1515</td>
<td>GE Research – Andrew Detor</td>
</tr>
<tr>
<td>1530</td>
<td>Univ Mass – Lowell – Alireza Amirkhizi (or alternate)</td>
</tr>
<tr>
<td>1545</td>
<td>Carnegie Mellon Univ – Aarti Singh</td>
</tr>
<tr>
<td>1600</td>
<td>Day 1 Wrap-up – Haines/Mallick</td>
</tr>
<tr>
<td>1630</td>
<td>Adjourn</td>
</tr>
</tbody>
</table>
AGENDA – DAY 2

Day 2 - Wednesday, July 13

1300  Welcome and charge for the day
1315  Purdue Univ – Alejandro Strachan
1330  Cal Tech Univ -Kaushik Bhattacharya
1345  Johns Hopkins Univ – KT Ramesh
1400  Data Management OV – Rinderspacher
1430  Johns Hopkins Univ – David Elbert
1445  Contextualize – Brandon Kappes
1500  Intro to Internal HTMDEC programs & why so important (‘C in CA’) – Haines/Mallick
1530  DEVCOM-ARL - Daniel Casem
1545  DEVCOM-ARL - Muge Fermen-Coker
1600  Day 2 Wrap-up - Discussion/Questions - ALL
1645  Adjourn
WHERE ARE WE GOING? ENDGAME

Program Goal: Develop the methodologies, models, algorithms, synthesis & processing techniques, and characterization methods to rapidly accelerate the discovery of novel materials for extreme conditions.
The overarching goal of this program is to couple automation and machine learning techniques to material manufacturing and characterization to demonstrate new materials that withstand and perform under extreme conditions. The program will develop the necessary methodologies, models, algorithms, synthesis & processing techniques, and requisite characterization and testing to rapidly accelerate the discovery of novel materials through data-driven approaches. As such, it is expected the results of this program will be the above techniques as well as novel materials exhibiting unprecedented properties at the appropriate scales that have been developed utilizing all of the aforementioned tools which will be provided to DEVCOM-ARL for further analysis and testing.

- New Methodologies
- New Models
- New ML algorithms
- New HT Synthesis & Processing Techniques
- New HT Characterization & Testing Techniques

Next gen materials for extreme conditions, discovered at an accelerated pace
PURPOSE OF THIS KICKOFF MEETING

1. Formal start to the program (after a long wait)

2. Layout program goals, expectations, and “calendar”

3. Allow all awardees to introduce their seedling programs, not only to each other, but ARL researchers

4. Encourage *early* interaction between awardees
   
   i. Hmm, we’re taking a different, but parallel approach…
   
   ii. Interesting, I really think we could help with that
   
   iii. We have great characterization & modeling, but could use their synthesis & processing
   
   iv. I wonder if they have considered using x, y, and z
   
   v. We’ve been looking for someone working in that area, we should definitely connect
FIRST & FOREMOST, CONGRATULATIONS!!

This was an extremely competitive process, and if you are here, you were in the top 10% of all applicants.

White Papers Submitted: 120+

Full Proposal Invites: 26

Awardees: 11 (9 General + 2 Data Mgmt)
HTMDEC TIMELINE – ‘TWAS A LONG ONE!

Materials Discovery Workshop held virtually: October 2020

FOA Draft to Legal & ACC for Input: Jan 2021

Pre-Solicitation release: June 2021

HTMDEC website goes live: 29 June 2021

Final Opportunity release: July 2021

FOA Opportunity Workshop: 29 July 2021

Deadline for Questions on Funding Opportunity: 6 August 2021

Whitepapers Due: 31 August 2021

Invitations for Proposals: October 2021

Proposals due: 1 November 2021

Seedling Awards: Jan 2022 - July 2022
AWARDEE DISTRIBUTION - GEOGRAPHICAL

- General Thrusts
- Data Management
AWARDEES BY INSTITUTION

Investigators by Institution
PROGRAM THRUST AREAS

There are two (2) FY22-specific thrust areas that will only be advertised in Year 1 of the FOA. The intent is to allow for effective teaming, program development, establishing a workflow (2022-1) and demonstration of a data handling & management platform that will be utilized throughout the program (2022-2).

FY2022-1 - Program & Workflow Development
FY2022-2 – Data Handling & Management

1. **Data-driven Material Design** - all aspects of the material design phase in the material development cycle which are accelerated through the integration of computational methods.

2. **High-Throughput Synthesis & Processing** – both modifying existing synthesis & processing methods to accommodate for high-throughput, as well as developing novel techniques.

3. **High-Throughput Characterization** – implementation of automation, as well as development of surrogate tests to mimic high-strain techniques which are not amenable to automation.

4. **ML-augmented Physics-Based Models** – integration of physics-based models with machine learning is poised to be a tipping point in materials science. To date, nearly all ML algorithms have been developed for big data (e.g. image recognition). We must discontinue ‘repurposing’ these algorithms and develop ML algorithms specifically designed for materials discovery, and informed by physics.
PROPOSAL THRUST AREAS

Targeted Thrust Areas (FY22 Only):

Texas A&M

Center

Data

JHU (Elbert et al.) Contextualize Inc.

General Thrust Areas:

Synthesis

Design

Modeling

Characterization

UCSD

Carnegie Mellon UMass Lowell

Georgia Tech UMass Lowell Purdue

JHU (Ramesh et al.) Caltech GE Research
We want awardees in different thrust areas to collaborate.
HTMDEC WEBSITE

https://arl.army.mil/HTMDEC

Program Description

Purpose: Within the Army science and technology enterprise, DEVCOM-ARL is chartered to conduct disruptive foundational research, engage as the Army’s primary collaborative link to the scientific community, and interface to shape future fighting concepts. We crystallize these ideas and the impetus to perform these functions at the pace of innovation as ‘Operationalize Science for Transformational Overmatch’. Simply put, we seek to accelerate discovery and transition breakthroughs to the Warfighter.

Rule-based artificial intelligence (AI) and machine learning (ML) tools present powerful avenues for exploring an information landscape in discovering novel materials for applications in extreme...
AS A REMINDER, HTMDEC IS NOT...

• A continuation of our previous CRA (Materials for Extreme Dynamic Environments - MEDE) – This is a brand new initiative, with many changes

• A program with a rigid structure for the next 5-10 years – we will be a dynamic program pivoting on the fly as the R&D develops

• ICME 2.0 – While ICME will likely play a role in any HT program, the focus is not to optimize the ICME methodology, but to extend HT processes through the entire lifecycle of materials development

• A program looking to merely recycle existing ML algorithms and models that have been developed for big data – Materials as a whole is a relatively sparse data set, materials for extreme conditions even more sparse. We realize a 1 yr Seedling may need to use existing algorithms and models, but we will expect more from multi-year Centers

• A program with the intent of **only** developing new “tools” (algorithms, models, synthesis and characterization techniques, characterization techniques – **novel materials** using these tools is essential to the success of this program
HTMDEC - NEW DIRECTIONS

• Previous CRAs
  – Advertised via Broad Agency Announcement (BAA)
  – Large ‘Center’ from the onset of program
  – One major, multi-year contract with multiple co-PIs (MURI model)
  – Limited flexibility for Government to run an agile program

• HTMDEC
  – Advertised via Funding Opportunity Announcement (FOA)
  – Awarded via multiple Cooperative Agreements (CAs)
  – Program initiates with numerous ‘Seedlings’, down-select to a few ‘Centers’ (closer to DARPA model)
  – Seedlings are of limited duration. They are expected to matriculate into part of a center (success) or terminate.
  – Centers + Seedlings in out-years, successful seedlings can be rolled into Centers
  – All participants are expected to participate in collaboration events; this will be one of the mechanisms for interaction between seeds, interactions with the WMR workforce and development of centers.
  – Encourages workforce development by offering Fellowships for graduate students who are US Citizens (in Centers)
# Seedling & Center Concept

**Seedling** – single year, narrowly focused (1 or 2 thrust areas) effort

**Center** – multiple year effort, comprehensive effort (must address all 4 thrust areas).

<table>
<thead>
<tr>
<th>Notional Tasks</th>
<th>Year 1</th>
<th>Year 2</th>
<th>Year 3</th>
<th>Year 4</th>
<th>Year 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data-Driven Material Design</td>
<td><img src="data-driven_diagram.png" alt="Diagram" /></td>
<td><img src="data-driven_diagram.png" alt="Diagram" /></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>High Throughput Synthesis &amp; Processing</td>
<td><img src="high-throughput_diagram.png" alt="Diagram" /> x 2-3</td>
<td><img src="high-throughput_diagram.png" alt="Diagram" /></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>High Throughput Characterization</td>
<td><img src="characterization_diagram.png" alt="Diagram" /></td>
<td><img src="characterization_diagram.png" alt="Diagram" /></td>
<td><img src="characterization_diagram.png" alt="Diagram" /></td>
<td><img src="characterization_diagram.png" alt="Diagram" /></td>
<td><img src="characterization_diagram.png" alt="Diagram" /></td>
</tr>
<tr>
<td>Physics-Based Model Informed ML</td>
<td><img src="physics-based_diagram.png" alt="Diagram" /></td>
<td><img src="physics-based_diagram.png" alt="Diagram" /></td>
<td><img src="physics-based_diagram.png" alt="Diagram" /></td>
<td><img src="physics-based_diagram.png" alt="Diagram" /></td>
<td><img src="physics-based_diagram.png" alt="Diagram" /></td>
</tr>
</tbody>
</table>
NOTIONAL CALENDAR

Fully Executed Awards: early July 2022

TBD – “Speed Dating”, Quarterly Review, Side Meeting at a Major Conference?

Program Review Meeting: early Apr 2023

Center Full Proposals Due: late May 2023

Proposal Reviews: early June 2023

Awardee Selections: mid June 2023

Center Awards: July 2023
**ANTICIPATED* PROGRAM STRUCTURE – YR 2+**

<table>
<thead>
<tr>
<th>Available Funding (yearly):</th>
<th>$5.7M</th>
</tr>
</thead>
<tbody>
<tr>
<td>Centers (2 or 3):</td>
<td>$4.0M</td>
</tr>
<tr>
<td>Seedlings (1-2):</td>
<td>$500K</td>
</tr>
<tr>
<td>Data Mgm’t Seedling:</td>
<td>$300K</td>
</tr>
<tr>
<td>ARL Internal Programs:</td>
<td>$900K</td>
</tr>
</tbody>
</table>

* All funding levels are approximate and depend on the approved Congressional budget.
ARL-INTERNAL HTMDEC PROJECTS

In order to promote fruitful collaborations between ARL and University partners, we have decided to run an internal proposal process in conjunction with the extramural process. The white paper/full proposal process, as well as program reviews, will run in parallel to assure selection of internal projects with strong alignment with the Centers.

It is expected that PIs chosen for internal projects will foster concrete collaborations with University partners within the HTMDEC Centers and essentially become “champions” of this research at ARL. This will work to maximize the likelihood of technology adoption and transition over time. Yearly program reviews will present an optimal opportunity to build these partnerships.

For Year 1, since no Centers have been chosen, we are funding projects which look to rapidly develop technologies that augment ARL’s HT capabilities.
PROPOSAL PROCESS

Final FOA Release: Mid July
Applicant’s Workshop: 29 JUL
White Paper Submission: 31 AUG
WP Reviews: SEP

FP Reviews: 8-19 NOV*
Full Proposal Submission: 1 NOV
Invite Full Proposals from Top WPs

Selections Announced: DEC

CAs Awarded: JUL ‘22

JUL ‘22
INTERNAL PROPOSAL PROCESS

- **SoN (off cycle)**: Late June
- **Information Session**: 22 July
- **White Paper Submission**: 31 August
- **WP Reviews**: September
- **Selections Announced**: 24 November
- **FP Reviews**: 8-19 November
- **Full Proposal Submission**: 1 November
- **Invite Full Proposals from Top WPs**: 1 October
- **Funding Released**: July 22
WORKFORCE DEVELOPMENT

- This CRA plans on putting a major focus on workforce development

- US Army wants the best & brightest from their University collaborators, and Universities want their students landing rewarding jobs, so this is a win-win

- We will be incentivizing using US graduate students in the HTMDEC program by providing program “fellowships” to Centers in the form of “plus up” funding for Professors who utilize US graduate students

- The intent of these fellowships is to maximize the likelihood of bringing much needed talent into ARL that will be savvy in both material science and data science (ML/AI), clearly the future of materials science

- Actual fellowship amounts and the details are still being determined