



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

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CAM, Deputy CAM, ST-Terminal Ballistics
WMRD

Approved for public release; distribution is
unlimited.



AGENDA – DAY 1



- 1300 *Welcome and Introductory Remarks*
- 1315 *Army Research Lab Executive Greeting*
- 1330 *HTMDEC OV & Program "Calendar" – Haines/Mallick*
- 1415 *Texas A&M Univ – Raymundo Arroyave (or alternate)*
- 1430 *Georgia Tech Univ – Surya Kalidindi (or alternate)*
- 1445 *Univ California San Diego – Kenneth Vecchio*
- 1500 *Break*
- 1515 *GE Research – Andrew Detor*
- 1530 *Univ Mass – Lowell – Alireza Amirkhizi (or alternate)*
- 1545 *Carnegie Mellon Univ – Aarti Singh*
- 1600 *Day 1 Wrap-up – Haines/Mallick*
- 1630 *Adjourn*



AGENDA – DAY 2



Day 2 - Wednesday, July 13

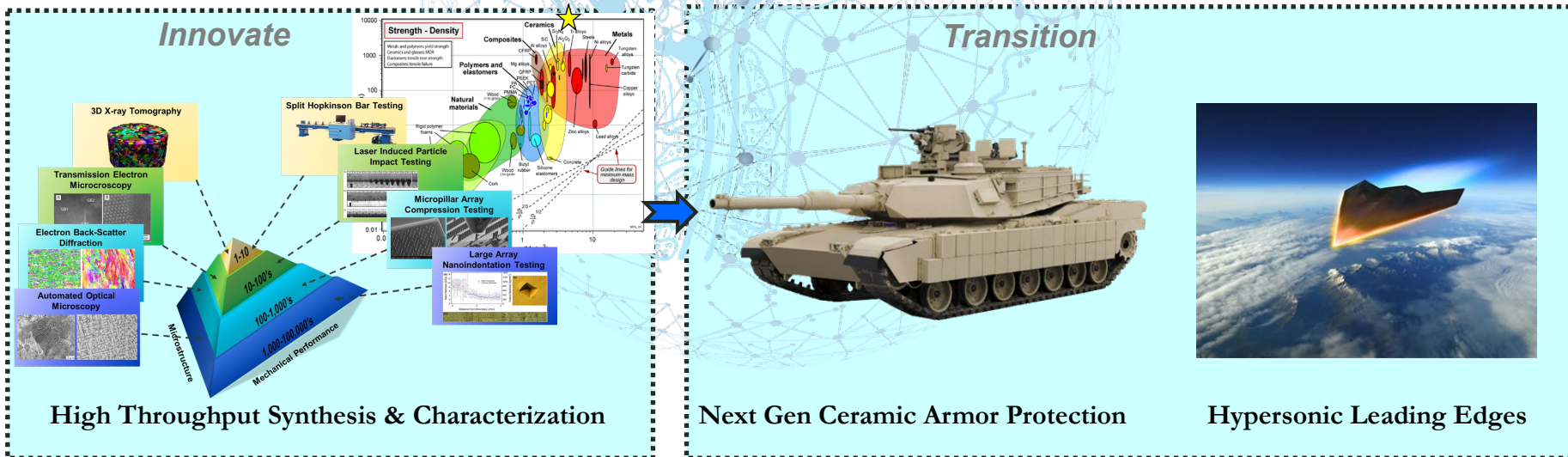
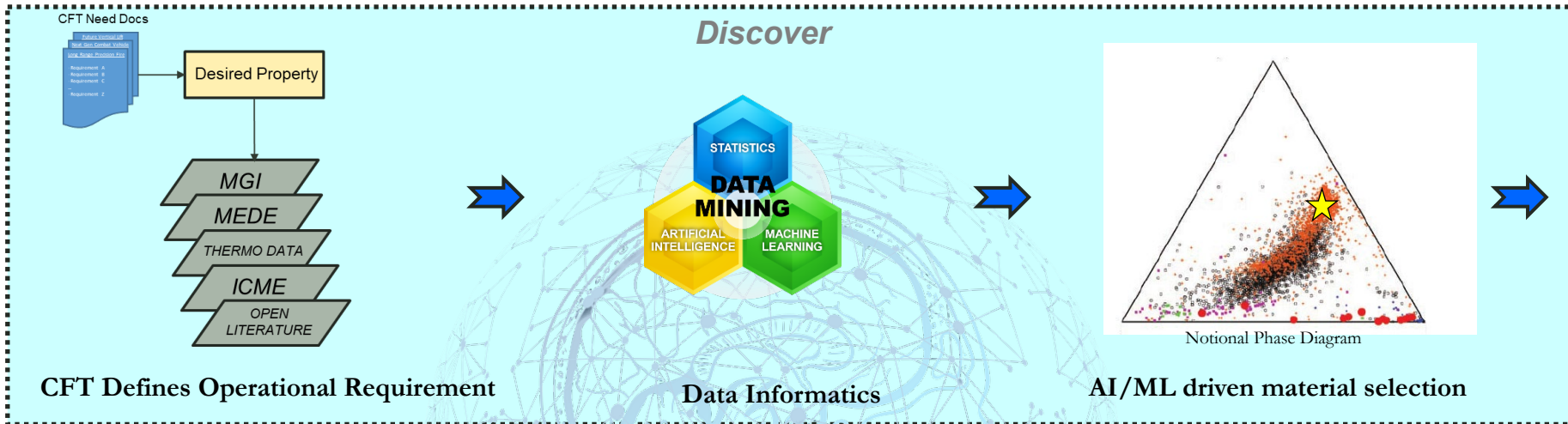
- 1300 *Welcome and charge for the day*
- 1315 *Purdue Univ – Alejandro Strachan*
- 1330 *Cal Tech Univ -Kaushik Bhattacharya*
- 1345 *Johns Hopkins Univ – KT Ramesh*
- 1400 *Data Management OV – Rinderspacher*
- 1430 *Johns Hopkins Univ – David Elbert*
- 1445 *Contextualize – Brandon Kappes*
- 1500 *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.





WHAT HTMDEC IS...



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 – ‘T WAS A LONG ONE!

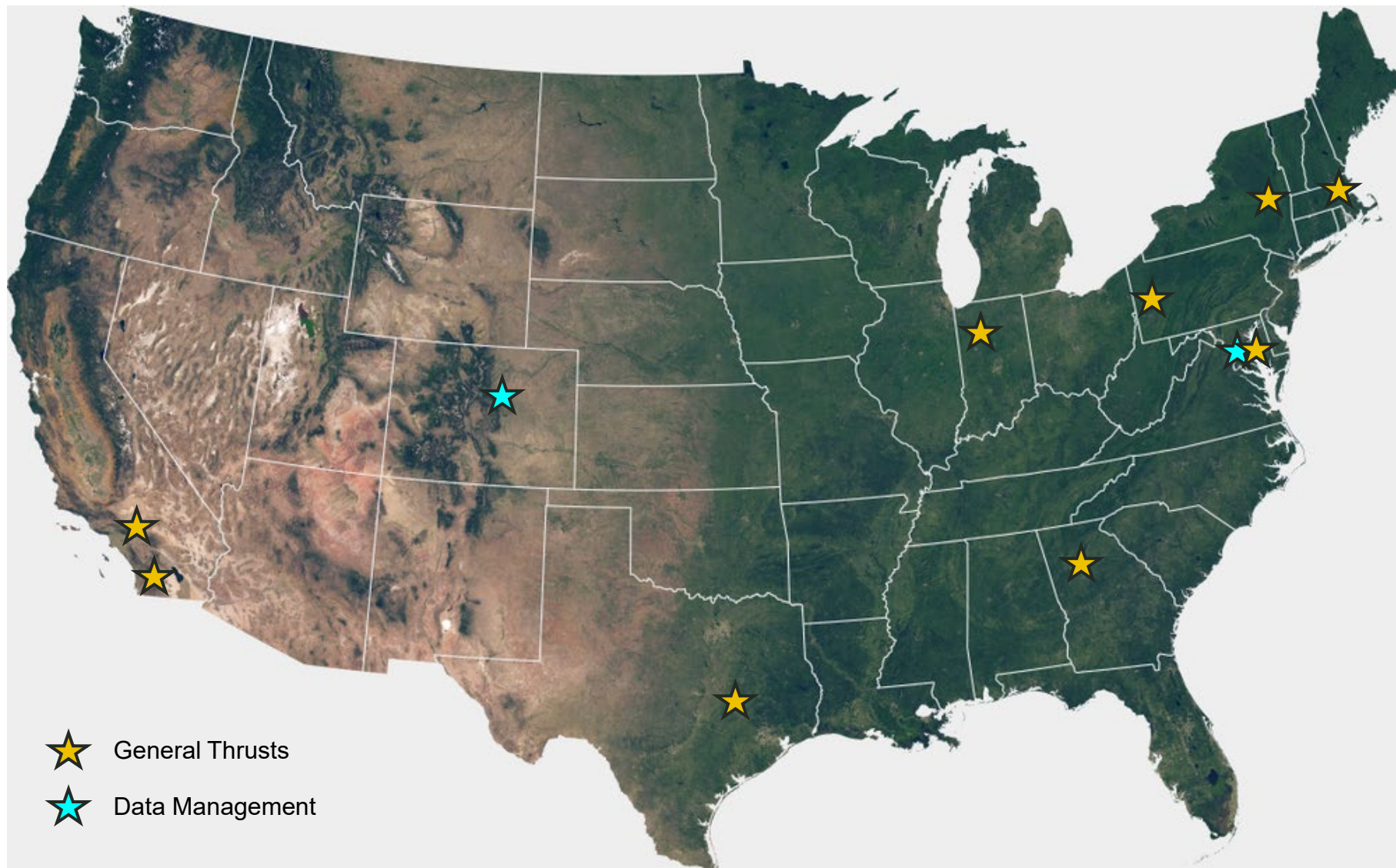


Materials Discovery Workshop held virtually	October 2020	✓
FOA Draft to Legal & ACC for Input	Jan 2021	✓
Pre-Solicitation release	June 2021	✓
HTMDEC website goes live	29 June 2021	✓
Final Opportunity release	July 2021	✓
FOA Opportunity Workshop	29 July 2021	✓
Deadline for Questions on Funding Opportunity	6 August 202	✓
Whitepapers Due	31 August 2021	✓
Invitations for Proposals	October 2021	✓
Proposals due	1 November 2021	✓
Seedling Awards	Jan 2022 July 2022	✓





AWARDEE DISTRIBUTION - GEOGRAPHICAL

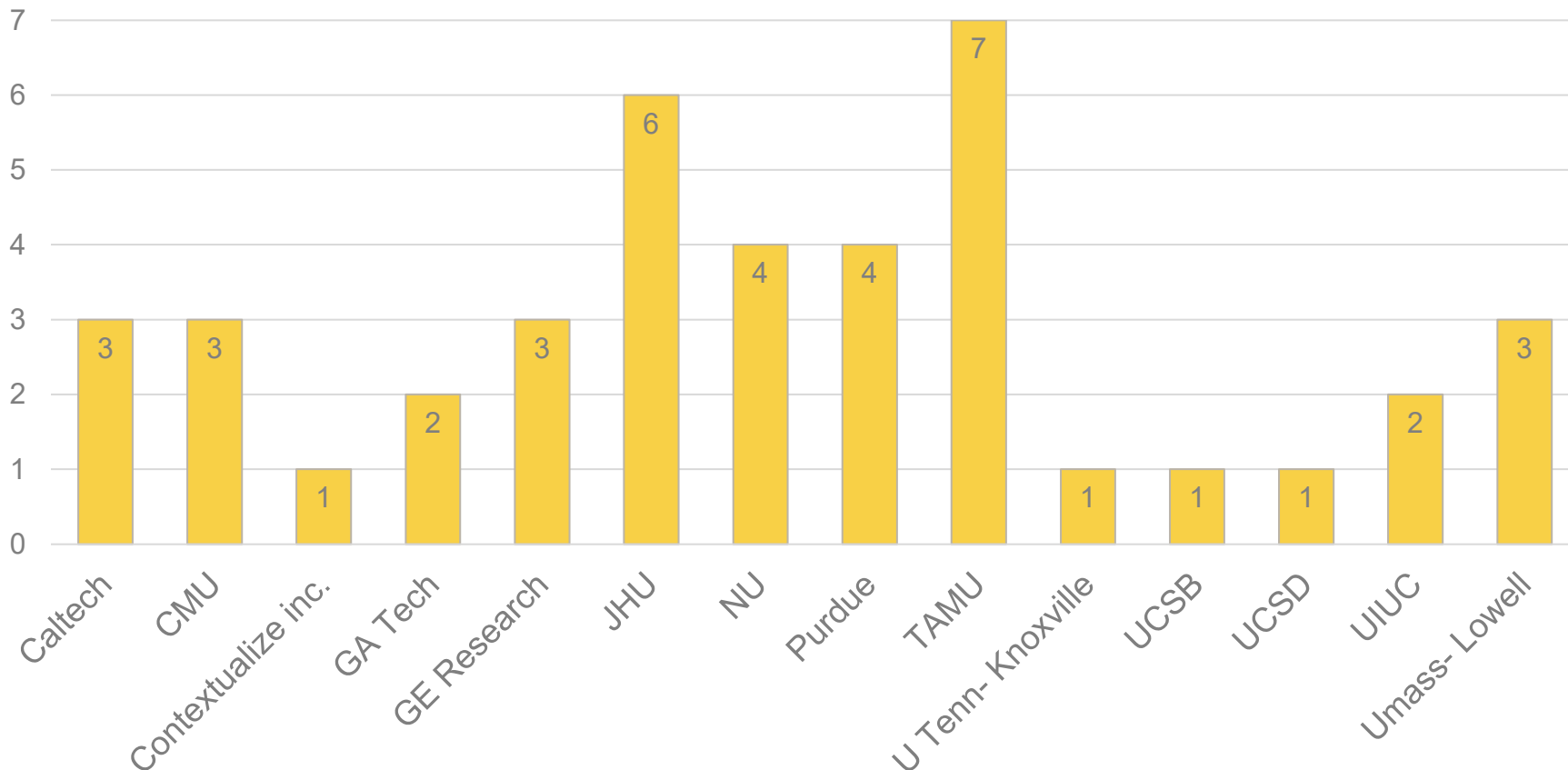




AWARDEES BY INSTITUTION



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

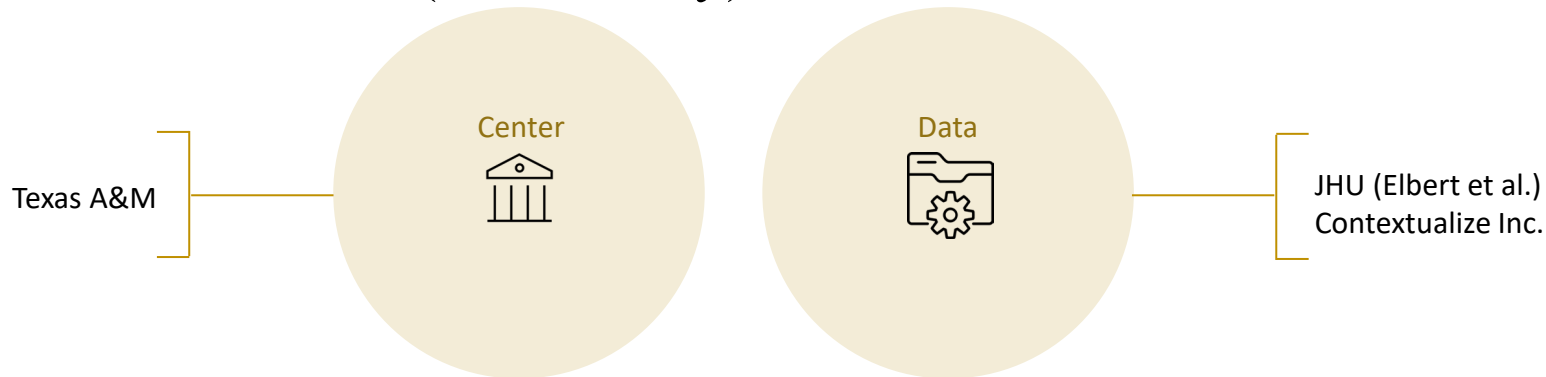
- 1. Data-driven Material Design** - all aspects of the material design phase in the material development cycle which are accelerated through the integration of computational methods.
- 2. High-Throughput Synthesis & Processing** – both modifying existing synthesis & processing methods to accommodate 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.



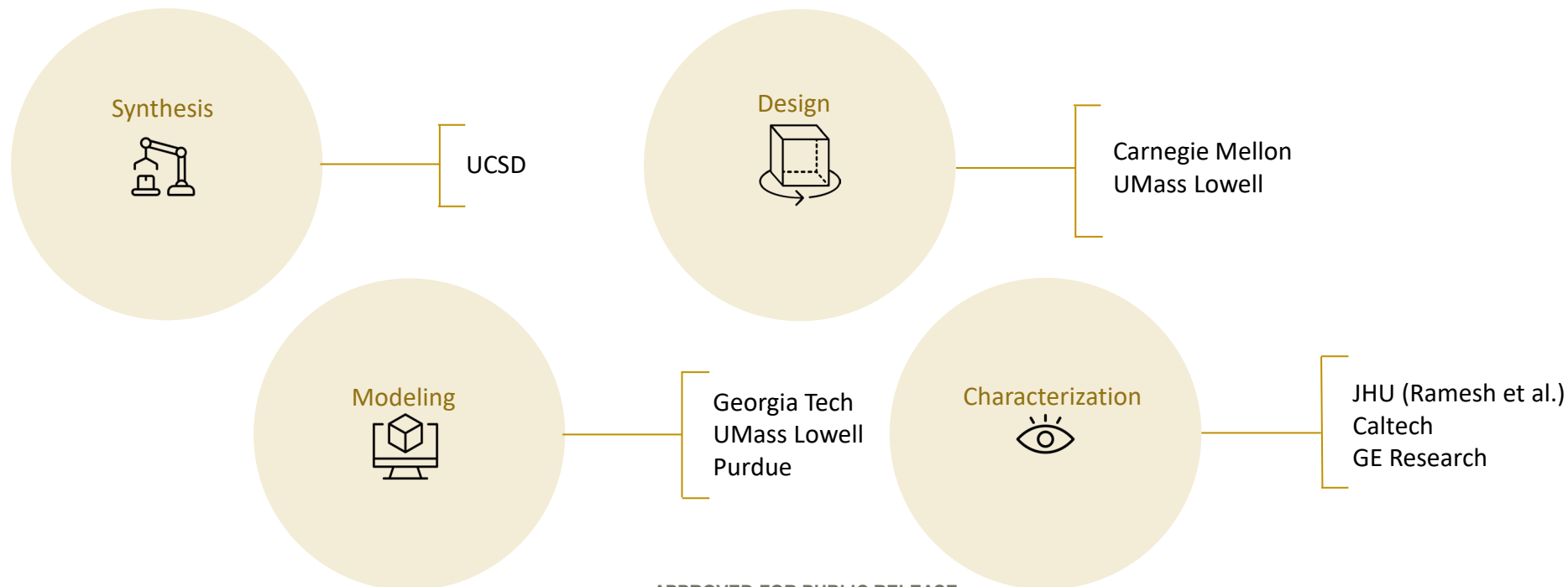
PROPOSAL THRUST AREAS



Targeted Thrust Areas (FY22 Only):

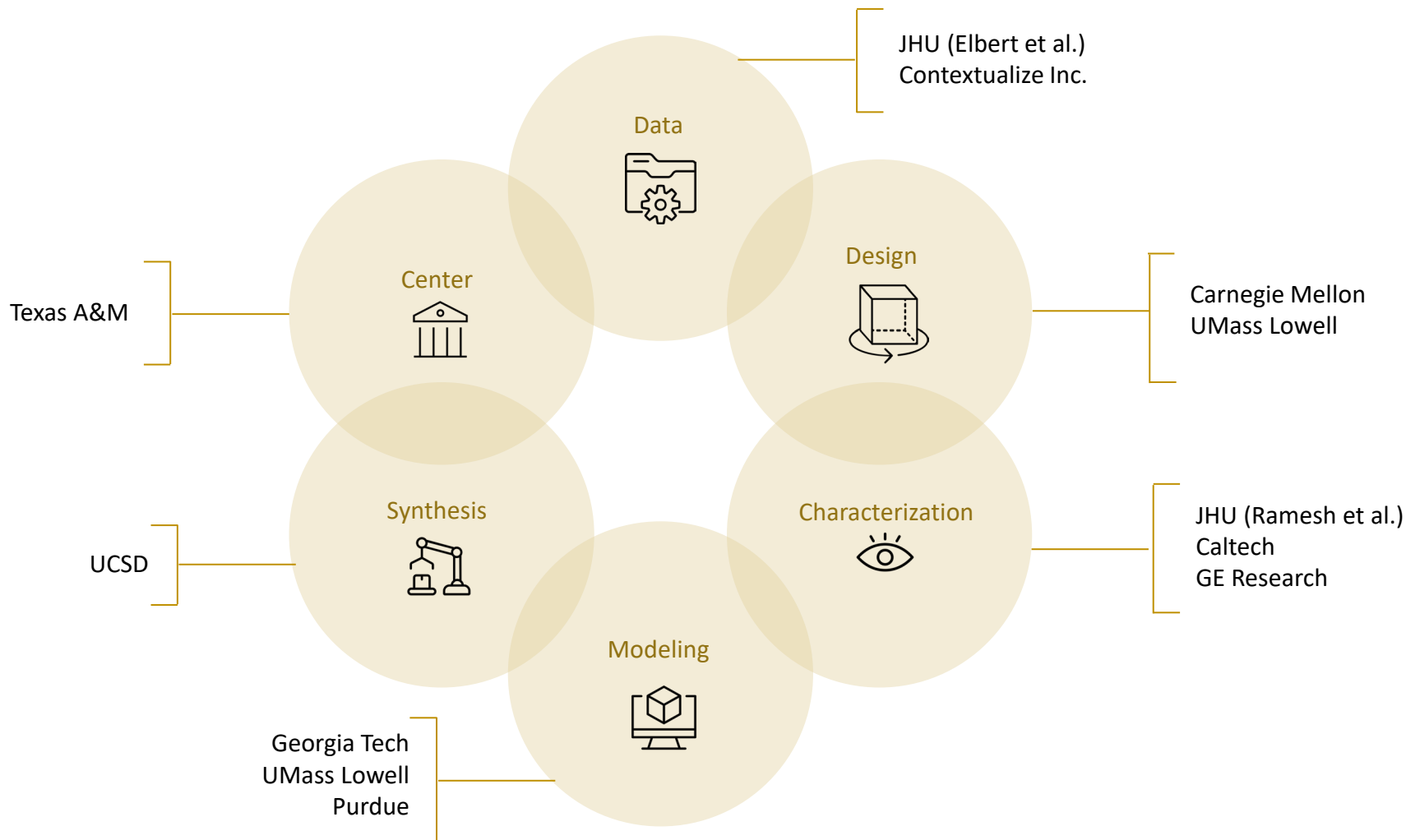


General Thrust Areas:





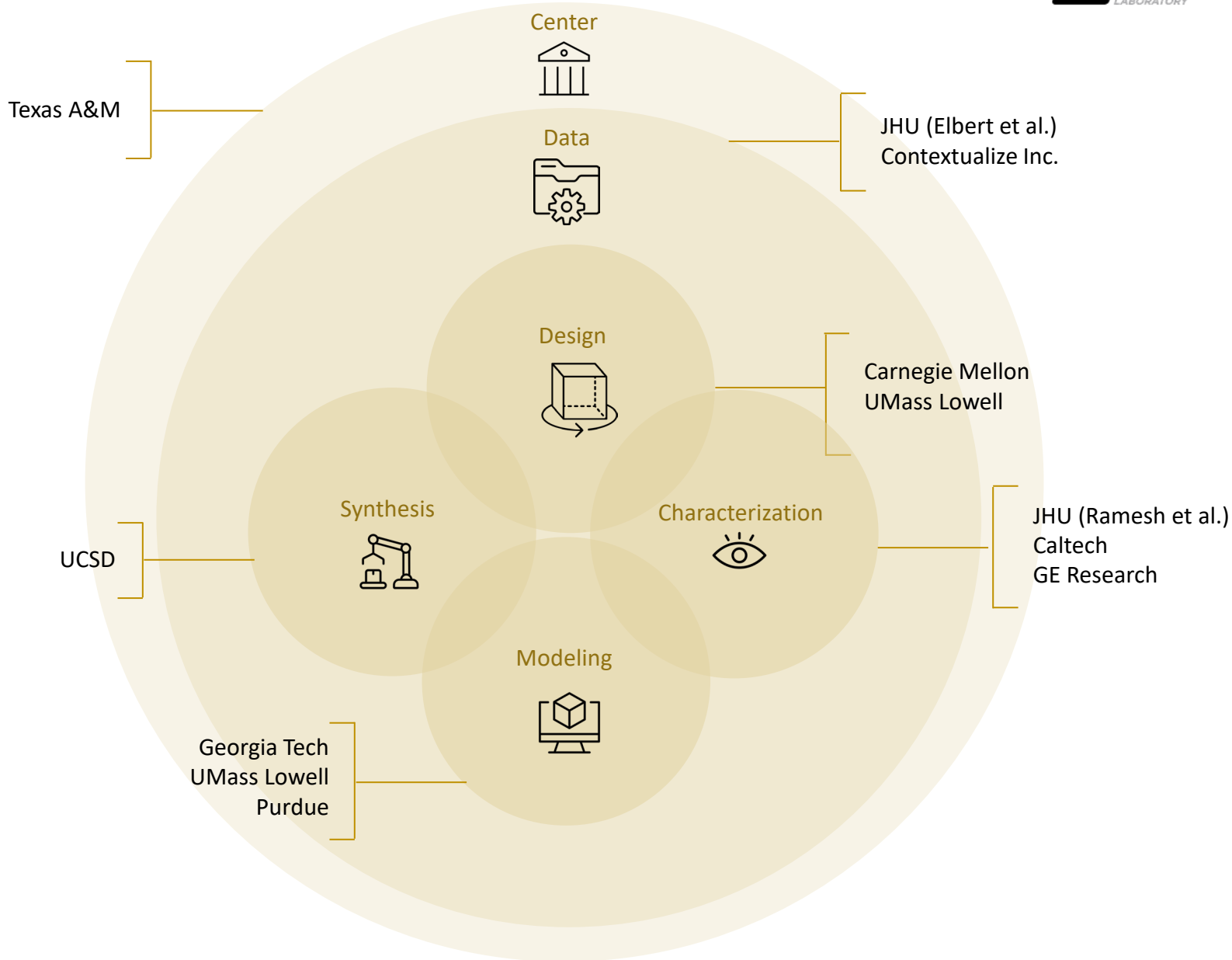
OUR OBJECTIVE: COLLABORATION



We want awardees in different thrust areas to collaborate.



IDEAL HIERARCHY OF THRUSTS:





HTMDEC WEBSITE



<https://arl.army.mil/HTMDEC>

High-Throughput Materials Discovery for Extreme Conditions (HTMDEC)

U.S. ARMY COMBAT CAPABILITIES DEVELOPMENT COMMAND ARMY RESEARCH LABORATORY
THE ARMY'S NATIONAL RESEARCH LABORATORY

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HIGH-THROUGHPUT MATERIALS DISCOVERY FOR EXTREME CONDITIONS (HTMDEC)

2021 HTMDEC APPLICANTS' DAY

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 crystalize 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

87°F Sunny 11:14 AM 7/14/2021

Special thanks to Jenna Brady and her team for their support



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)

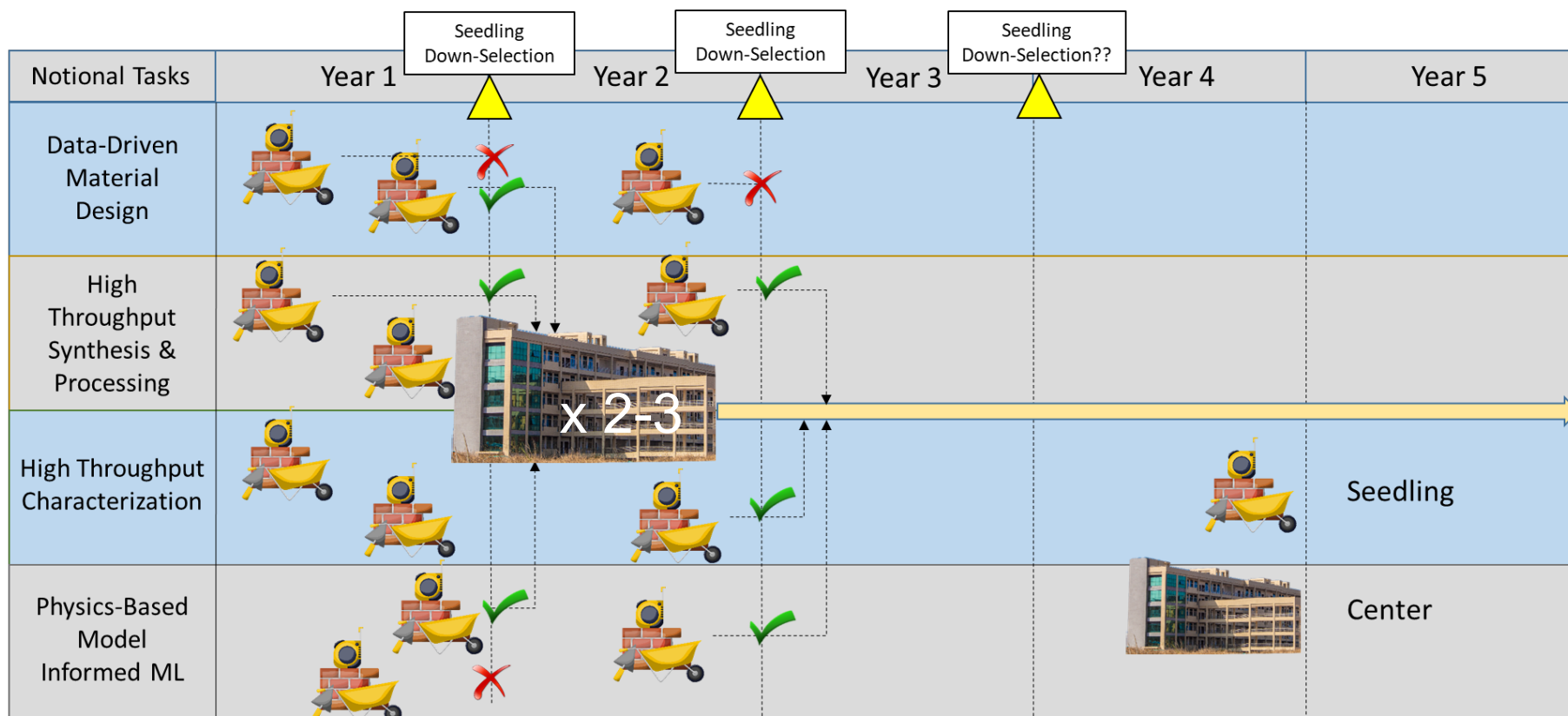


SEEDLING & CENTER CONCEPT



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

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





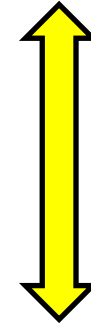
NOTIONAL CALENDAR



Fully Executed Awards

early July 2022 

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



9 months

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+



Available Funding (yearly):	\$5.7M
Centers (2 or 3):	\$4.0M
Seedlings (1-2):	\$500K
Data Mgm't Seedling:	\$300K
ARL Internal Programs:	\$900K

* All funding levels are approximate and depend on the approved Congressional budget.



ARL-INTERNAL HTMDEC PROJECTS



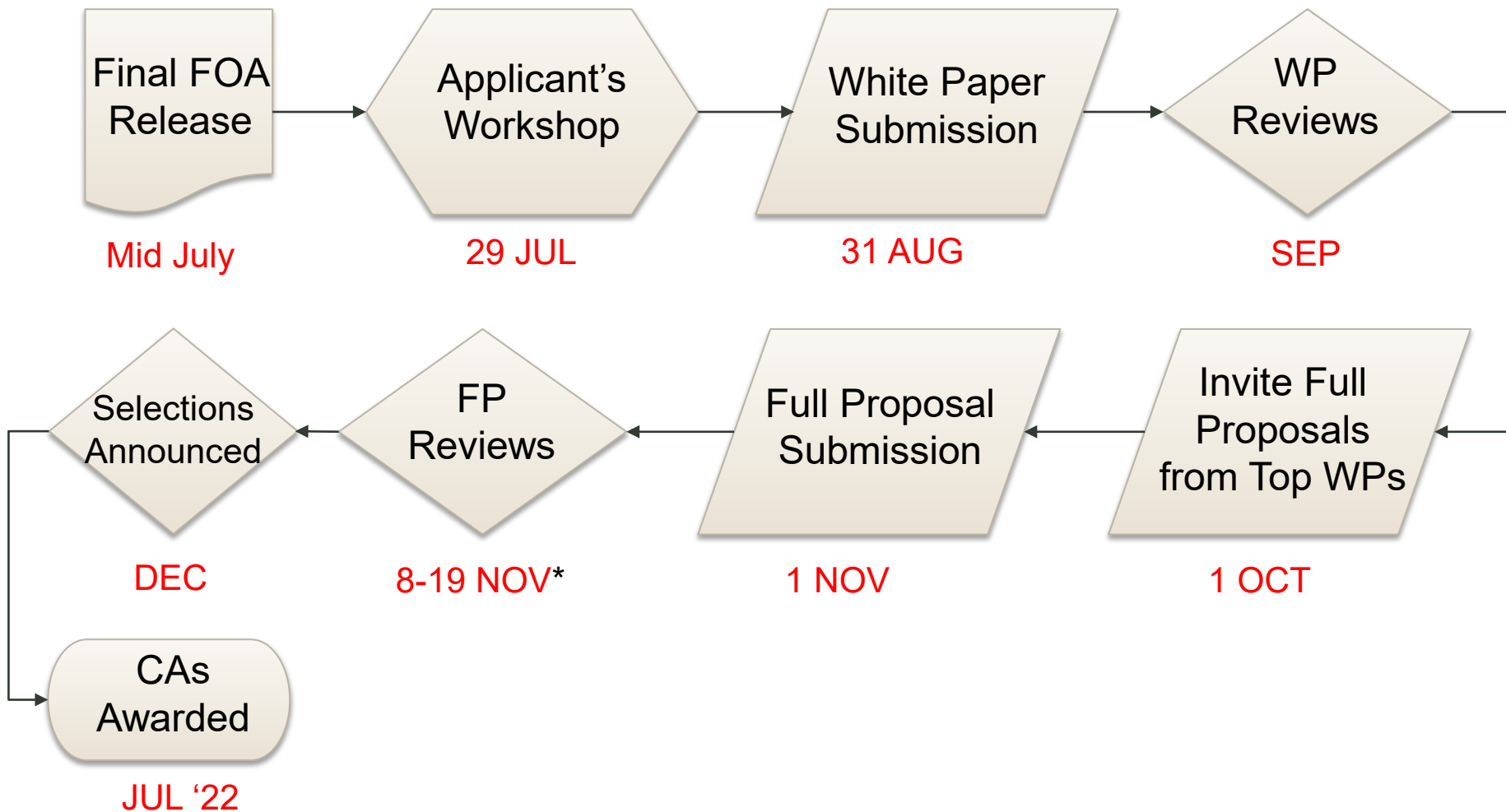
In order to promote fruitful collaborations between ARL and University partners, we have decided to run an internal proposal process in conjunction with the extramural process. The white paper/full proposal process, as well as program reviews, will run in parallel to assure selection of internal projects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

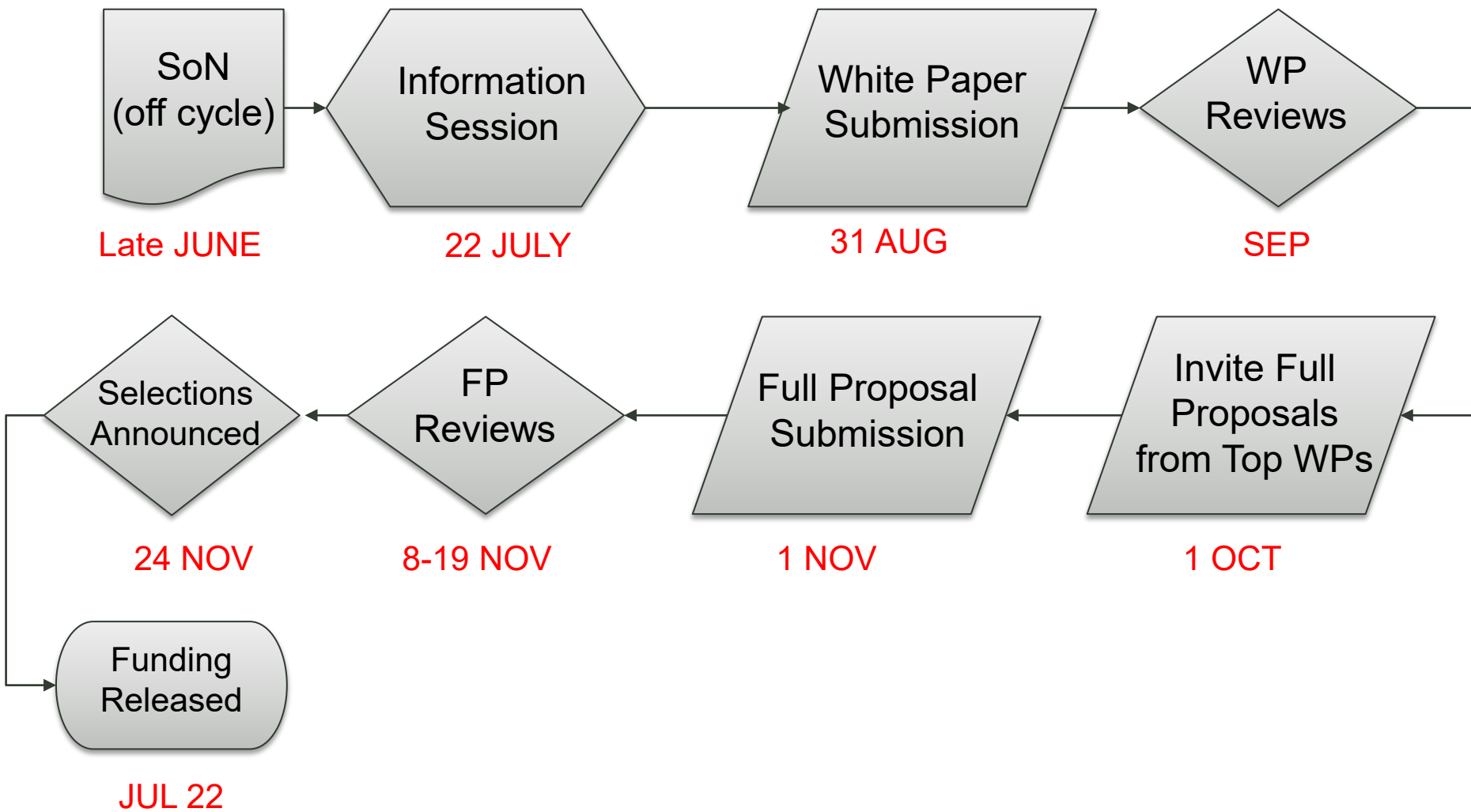


PROPOSAL PROCESS





INTERNAL PROPOSAL PROCESS





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