Microsystems Exploration Topic (μE)
DARPA-PA-21-05-02
Predictive Nanoscale Simulation for the Terahertz Regime (NanoSim)

I. Topic Description

The Defense Advanced Research Projects Agency (DARPA) is issuing a Microsystems Exploration topic (μE) inviting submissions of innovative basic or applied research concepts in the technical domain of predictive device simulation. This μE is issued under the Program Announcement for Microsystems Exploration, DARPA-PA-21-05. All proposals in response to the technical area(s) described herein will be submitted to DARPA-PA-21-05 and if selected, will result in an award of an Other Transaction (OT) for prototype project not to exceed $1,000,000.

To view the original DARPA Program Announcement for Microsystems Exploration visit SAM.gov under solicitation number DARPA-PA-21-05:
https://sam.gov/opp/ceea97241e8c4a77a11045fddb51ab82/view.

A. Introduction

State-of-the-art (SOA) technology computer aided design (TCAD) tools rely on simplifying assumptions to provide a simulation result in a reasonable amount of computational time, but are inaccurate for deeply-scaled devices, where the active regions consist of only a few thousand atoms and the interface and surface physics dominate material characteristics. In addition, when the device dimension is approaching, or smaller than, the carrier mean free path, highly non-equilibrium carrier energy distribution and non-quasi static stochastic transport must be factored into device modeling to accurately predict its fast transient characteristics and terahertz (THz) frequency behavior.

B. Objective/Scope

The NanoSim micro-exploration (μE) will develop accurate and computationally fast techniques to predict nanoscale material properties and apply the results to TCAD device design, enabling fast turn-around predictive modeling of nanoscale devices operating in the THz regime. To achieve computationally fast and accurate modeling of realistic devices composed of 1,000-10,000 atoms in a TCAD environment, NanoSim will explore the following novel technical approaches:

1. **Achieving 1000X acceleration of quantum modeling and simulation for predictive nanoscale electronic properties:** Recent research into direct quantum mechanical simulation of devices on the nanoscale has focused on Density-Functional Theory (DFT), a computational quantum mechanical modeling technique used in multiple scientific disciplines, to investigate the electronic structure of nanoscale structures. DFT is highly accurate, and more computational efficient than a Monte Carlo (MC) based approach, but still time consuming especially when solving a problem involving the interactions of a larger, 1000s of atoms system. Today, using DFT to solve a 100-atom system requires roughly 40 cores running in parallel for a week. NanoSim will explore approaches to accelerate DFT using approximate computing methods such as machine learning, partitioning, and fast stochastic sampling to provide a reduced set of possible solutions to significantly reduce the complexity of the

subsequent DFT computation, enabling a predictive deterministic solution while using significantly fewer computational resources over a much shorter timeframe. These innovations will enable a simulation speedup of greater than 1000X versus traditional DFT computation, producing a realistic solution within hours in a TCAD environment on a high-end workstation.

2. **Achieving accurate nanoscale device transport calculations for the THz regime:** With access to accurate materials and relevant electrical and interface parameters with realistic device geometries from technical approach number one, quantum-mechanical based transport methods such as the non-equilibrium Green's function, currently used for physics phenomena research, could be incorporated in a TCAD environment to describe picosecond transients and THz frequency behavior of nanoscale devices. Performers will develop such non-equilibrium, non-quasistatic transport equations with quantum mechanical-based scattering mechanisms, and incorporate them with accelerated computational techniques in device TCAD to accurately model nano-scale devices operating at THz speed with >95% accuracy when compared to published experimental results.

C. Structure

Proposals submitted to DARPA-PA-21-05-02 in response to the technical area of this μE topic must be UNCLASSIFIED and must address two independent and sequential project phases: a Phase 1 Feasibility Study (base) and a Phase 2 Proof of Concept (option). The period of performance for these phases are 9 months for the Phase 1 base effort and 9 months for the Phase 2 option effort. Combined Phase 1 base and Phase 2 option efforts for this μE topic should not exceed 18 months. The Phase 1 (base) award value should not exceed $500,000. The Phase 2 (option) award value should not exceed $500,000. The total award value for the combined Phase 1 and Phase 2 is limited to $1,000,000. This total value includes both Government award funding and any performer cost share, if required or proposed. Please review DARPA-PA-21-05 for requirements regarding cost share. Phase 1 studies will be evaluated to determine the feasibility of the approach and whether to exercise the Phase 2 option. Anticipated program will be 6.2. Therefore, research conducted by universities (prime or subcontractor) would be fundamental research and research conducted by all other organizations (prime or subcontractor) would be restricted research.

Proposals should clearly detail:

- The proposed predictive electronic properties modeling of complex nano-size devices with several materials and interfaces, and include any initial theory, simulations, or measured data to support model accuracy, scalability and performance claims.
- The proposed non-quasi static modeling approach and any initial theory, simulations, or measured data to support model accuracy, scalability and performance claims.
- The proposed approximate computing methods to accelerate the materials and the transports simulations and their accuracy and potential speed-ups.
- The proposed state of the art baseline material system(s) and device structure(s) to be investigated during the program, with current modeling results or measurements as references.
- Any new physics theory or mathematical techniques to be developed or leveraged by the program.
- Performer-defined goals (in addition to those defined in the Metrics Table below) and a

comparison with the current state-of-the-art technology.

- Simulation milestones from Phase 1 and Phase 2 along with their respective expected deliverables and schedule.
- Expected risks and risk mitigation strategies

The Government reserves the right to award all, some, one, or none of the options on the agreements(s) of the Phase 1 performers based on available funding, Phase 1 technical performance, and an assessment of the feasibility of the approach.

D. Technical Area Description

The NanoSim program consists of one technical area. Phase 1 (Feasibility Study) will focus on development of fast and accurate computational techniques to derive accurate nanoscale material properties and predictive THz and pico-second device electrical characteristics. Performers will first establish a baseline approach for rapid simulation of material structures where the properties are known and can be compared against recent published results. Next, performers will develop new rapid non-quasi static transport modeling techniques for the devices built on the baseline device material that accurately reproduce of the electrical performance, all with greatly decreased computational burden. Throughout this phase, performers will work to achieve higher degrees of modeling complexity, culminating in the accelerated simulation of nano-size structures that are formed from multiple material layers, and accurately produce the relevant material electronic properties for device applications. For carrier dynamic modeling, computational efficient techniques should focus on predicting electronic transport properties of nano-scaled systems including quantum mechanical transport properties and high frequency response. The primary criteria for successful completion of Phase 1 feasibility assessment will be to meet all Phase 1 NanoSim metrics, supported by theory, simulation results and published experimental measurements. In addition, data that supports the improved scalability of the non-quasi static material modeling approach in comparison to the baseline approach is required.

Phase 2 (Proof of Concept) will apply the time-efficient material properties and electronic transport simulation techniques developed in Phase 1 to model nanoscale devices under non-stationary, non-quasistatic transport conditions in a TCAD environment. Just as in Phase 1, performers will first establish a highly accelerated baseline approach for simulating scaled-up device structures compared to Phase 1, and where the properties are known and can be compared against recently published results. Next, performers will develop and apply their time-efficient non-quasi static transport modeling techniques for the scaled-up baseline material structures to accurately reproduce the baseline device high frequency and picosecond transient electrical characteristics, with greatly decreased computational burden. Throughout this phase performers will work to achieve higher degrees of modeling complexity, culminating in a highly time-efficient simulation of structures that are formed from multiple material layers and up to ten thousand atoms, for predictive device characteristics simulation. For device electrical performance modeling, the focus should be on predicting electronic transport properties of deeply scaled nano-size devices with over 95 % accuracy and high computational efficiency, and suitable for implementing in a TCAD framework. The primary criteria for the successful completion of Phase 2 (Proof of Concept) will be to meet all Phase 2 NanoSim metrics, supported by theory, simulation results and published experimental measurements. In addition, data that supports the improved scalability of the TCAD hosted computational efficient non-quasi static device modeling approach, in comparison to the baseline TCAD approach, is required.

Table 1. NanoSim Metrics*

NanoSim	Frequency (GHz)	Interacting Atoms in Simulation	Interacting Materials/ Interfaces Simulated	Number of devices simulated	Accuracy vs publication	Computational Speedup
Phase 1 Materials	≥100	Up to 1,000	≥2	N/A	≥95%	$\geq 10^3$ than SOA
Phase 2 Devices	≥250	Up to 10,000	≥3	≥3 (1,000 atom) ≥1 (10,000 atom)	≥95%	$\geq 10^4$ than SOA

***** Nominal values and should be refined by proposer based on proposer-defined device requirements

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E. Schedule/Milestones

Proposers must address the following Research Project Objectives, metrics, and deliverables, along with fixed payable milestones in their proposals. The task structure must be consistent across the proposed schedule, Task Description Document (TDD), and the Vol. 2 - Price Volume. If selected for award negotiation, the fixed payable milestones will be directly incorporated into Attachment 3 of the OT agreement ("Schedule of Milestones and Payments") with milestone amounts calculated based on the proposed accumulation of monthly amounts up to each milestone date. Please see the sample OT for Prototype provided as an attachment to DARPA-PA-21-05.

For planning and budgetary purposes, proposers should assume a program start date of **April 8, 2023.** Schedules will be synchronized across performers, as required, and monitored/revised as necessary throughout the program.

All proposals must include the following meetings and travel in the proposed schedule and costs:

- To foster collaboration between teams and disseminate program developments, a two-day Principal Investigator (PI) meeting will be held approximately every six months, with locations split between the East and West Coasts of the United States. For budgeting purposes, plan for three two-day meetings over the course of 18 months: two meetings in the Washington, D.C. area and one meeting in the San Francisco, CA area.
- Regular teleconference meetings will be scheduled with the Government team for progress reporting as well as problem identification and mitigation. Proposers should also anticipate at least one site visit per phase by the DARPA Program Manager during which they will have the opportunity to demonstrate progress towards agreed-upon milestones.

Fixed milestones for the program must include:

Month	Phase 1 Milestones
2	**Milestone 1:** Development of baseline material simulation, with >1000x acceleration compared to SOA approaches, for moderate complexity material structures, where the electronic properties are known and can be compared against published results. • Baseline material models structure properties should match recent published results to within 10%

	• Milestone Report should account for the differences in current SOA models vs the baseline approach
4	**Milestone 2:** Application of new computationally efficient non-quasi static modeling techniques to simulate moderate complexity material structures, where the electronic properties are known and can be compared against published results. • Device high frequency and fast transient behavior should match recent published results to within 5% • Milestone Report should account for the differences in new computational efficient models vs the baseline approaches including analysis of computational complexity and efficiency.
6	**Milestone 3:** Extension of the material simulation, with >1000x acceleration compared to SOA approaches, for moderate complexity material structures with 2 layer complexity and up to 1000 atoms. • Material structure property predictions should match current published results within 5%. • Milestone Report should focus on applying new highly accelerated techniques to predicting properties of nano-dimension systems with up to 1000 atoms, including meeting the Phase 1 NanoSim metrics, as well as plans to apply the models in a TCAD environment.
8	**Milestone 4:** Refinement of highly accelerated non-quasi static transport modeling techniques for high complexity material structures to match the electrical performance against current published results. • Milestone Report should focus on predicting high frequency and fast transient performance of nano-scaled devices including meeting all Phase 1 NanoSim metrics, as well as plans to apply these models in a TCAD environment.

Month	Phase 2 Milestones
10	**Milestone 5:** Development of highly accelerated baseline computational models for nanoscale material properties and device transport calculations in a TCAD environment. • Models should incorporate findings from Phase 1 material properties of moderate complexity, where the electronic properties are known and can be compared against published results, and the nano-dimension device high frequency and fast transient performance, where the electrical characteristics are known and can be compared against published results. • Accelerated models should be developed in an existing TCAD simulation environment. • Initial baseline model properties should match recent published results to within 5%. • Milestone Report should account for the differences in current SoA models vs the baseline approach.
12	**Milestone 6:** Application of proposed new highly accelerated computational techniques, to enhance modeling results of devices in terms of device dimension, interface properties, and material compositions. • Techniques should account for arbitrary changes in device geometry and boundary conditions, to predict electronic transport characteristics for multiple geometries (≥2) and up to 10,000 atoms, to within 5% of recent published results. • Milestone report should provide analysis that accounts for the differences in current SOA models vs the enhanced computational techniques developed.
14	**Milestone 7:** Acceleration of proposed new computational techniques to demonstrate scalability of approach in a TCAD environment. • Milestone Report analysis should demonstrate 1,000x speedup on a single high-performance workstation and demonstrate the potential for additional speedup consistent with future increases in computing capability.

16	**Milestone 8:** Demonstration of a highly accelerated integrated material and device TCAD simulation framework that can predict the high frequency and fast transient behavior of complex nano-dimension devices from first principles. • Techniques should meet all the Phase 2 metric. • Milestone Report analysis should account for the differences in current SOA models vs the enhanced computational techniques developed.
18	**Milestone 9:** Incorporation of new material and device computational techniques with existing TCAD to provide a standalone plugin capable of running simulations on a standalone workstation or cloud environment. • Milestone report detailing the operation of this standalone plug-in meeting all of the Phase 2 NanoSim metrics as well as NanoSim plugin code.

F. Deliverables

Performers will be expected to provide at a minimum the following deliverables:

- Key Phase 1 Deliverable: Written "End of Phase 1" milestone report and accompanying power point presentation to be presented one month prior to the end of phase (Month 8).
- Key Phase 2 Deliverables: Written "End of Phase 2" milestone report, accompanying power point presentation and TCAD plugins to accelerate modeling of materials for non-quasi static device transport property prediction.
- All additional milestone reports are assumed to be in power point presentation format with an accompanying presentation, every two months at the bimonthly milestone review telecon.
- Negotiated deliverables specific to the objectives of the individual efforts. These may include registered reports, experimental protocols, publications, intermediate and final versions of software libraries, code, and APIs, including documentation and user manuals, and/or a comprehensive assemblage of design documents, models, modeling data and results, and model validation data.

II. Award Information

Selected proposals that are successfully negotiated will result in award of an OT for prototype project. See Section 3 of DARPA-PA-21-05 for information on awards that may result from proposals submitted in response to this notice.

Proposers must review the model OT for Prototype agreement provided as an attachment to DARPA-PA-21-05 prior to submitting a proposal. DARPA has provided the model OT in order to expedite the negotiation and award process and ensure DARPA achieves the goal of Microsystems Exploration, which is to enable DARPA to initiate a new investment in less than ninety (90) days from each µE topic announcement. The model OT is representative of the terms and conditions that DARPA intends to award for all Microsystems Exploration Awards. The task description document, schedule of milestones and payments, and data rights assertions requested under Volumes 1, 2, and 3 will be included as attachments to the OT agreement upon negotiation and award.

As discussed in DARPA-PA-21-05, Section 5, "Application and Submission Information," proposers may suggest edits to the model OT for consideration by DARPA and provide a copy of the model OT with track changes as part of their proposal package. It is strongly encouraged that proposers include comments providing rationale for any suggested edits of a non-administrative nature. Suggested edits may be rejected at DARPA's discretion. **In order to ensure that DARPA achieves the Microsystem Exploration goal of award within 90 days from the posting date of the µE topic announcement, DARPA reserves the right to cease negotiations if the parties fail to reach agreement on OT award terms and conditions within this time period (on or before April 8, 2023).** If edits to the model OT are not provided as part of the proposal package, DARPA assumes that the proposer has reviewed and accepted the award terms and conditions to which they may have to adhere and the sample OT agreement provided as an attachment, indicating agreement with the listed terms and conditions applicable to the specific award instrument.

III. Eligibility

See Section 4 of DARPA-PA-21-05 for information on who may be eligible to respond to this notice.

IV. µE Topic Responses

Responses to this µE topic must be submitted as full proposals to DARPA-PA-21-05 as described therein. All proposals must be unclassified.

A. Proposal Content and Format

All proposals submitted in response to this notice must comply with the content and format instructions in Section 5 of DARPA-PA-21-05. All proposals must use the templates provided as Attachments to the PA and follow the instructions therein.

Information not explicitly requested in DARPA-PA-21-05, its Attachments, or this notice may not be evaluated.

B. Proposal Submission Instructions

See Section 5 of DARPA-PA-21-05 for proposal submission instructions.

C. Proposal Due Date and Time

Proposals in response to this notice are due no later than 4:00 p.m. Eastern on **February 7, 2023**. Full proposal packages as described in Section 5 of DARPA-PA-21-05 must be submitted per the instructions outlined therein *and received by DARPA* no later than the above time and date. Proposals received after this time and date may not be reviewed.

Proposers are warned that the proposal deadline outlined herein is in Eastern Time and will be strictly enforced. When planning a response to this notice, proposers should take into account that some parts of the submission process may take from one business day to one month to complete (e.g., registering for Unique Entity ID or TIN, renewing entity registration in SAM.gov).

V. Proposal Evaluation and Selection

Proposals will be evaluated and selected in accordance with Section 6 of DARPA-PA-21-05. Proposers will be notified of the results of this process as described in Section 7.1 of DARPA-PA-21-05.

VI. Administrative and National Policy Requirements

Section 7.2 of DARPA-PA-21-05 provides information on Administrative and National Policy Requirements that may be applicable for proposal submission as well as performance under an award.

VII. Point of Contact Information

Jason Woo, Program Manager, DARPA/MTO, NanoSim@darpa.mil

VIII. Frequently Asked Questions (FAQs)

All technical, contractual, and administrative questions regarding this notice must be emailed to NanoSim@darpa.mil. Emails sent directly to the Program Manager or any other address may result in delayed or no response.

All questions must be in English and must include name, email address, and the telephone number of a point of contact. DARPA will attempt to answer questions publically in a timely manner; however, questions submitted within seven (7) days of the proposal due date listed herein may not be answered.

DARPA will post an FAQ list under the µE topic on the DARPA/MTO Opportunities page at (http://www.darpa.mil/work-with-us/opportunities) The list will be updated on an ongoing basis until one week prior to the proposal due date. In addition to the FAQ specific to this notice, proposers should also review the Program Announcement for Microsystems Exploration General FAQ list on the DARPA/MTO Opportunities page under the Program Announcement (DARPA-PA-21-05).

To aid in the proposal preparation process, a Proposal Preparation Checklist and Tips document has been provided with the µE topic announcement on sam.gov. This document can also be found along with the FAQ posted on the DARPA/MTO Opportunities page at (http://www.darpa.mil/work-with-us/opportunities).