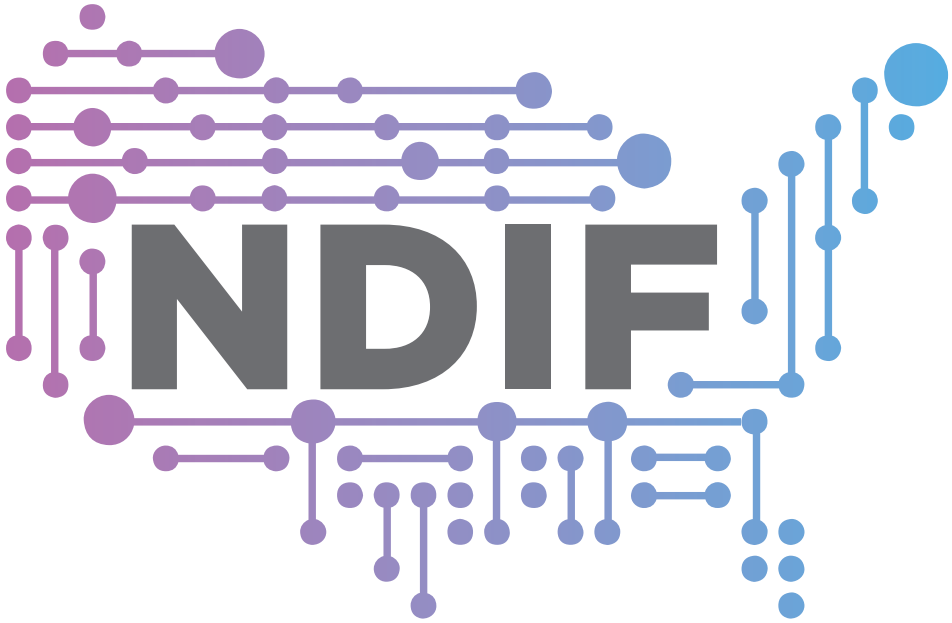
National Deep Inference Facility for Very Large Language Models (NDIF)

Project Proposal to the NSF

November 2023



1 A Computational Microscope for Large Language Models

Powerful large language models (LLMs) such as ChatGPT [1] herald a new era of artificial intelligence (AI) that is poised to reshape society [2], but *scientists cannot explain their predictions*. LLMs are able to write cogently about real-world topics [3], follow human instructions [4], and even pass legal [5], medical [6], and computer programming [7] exams. Both policymakers [8] and researchers [9] have stressed the urgency of explaining *how* they perform such tasks.

Because we know how to *create* LLMs, we can clearly envision the instrumentation necessary to open up their black-box calculations and *explain* them. **Just as physicists characterize particles using atom smashers and biologists catalog genes using DNA sequencers, researchers will explain machine intelligence by running LLMs under a computational microscope.** If we continue to deploy LLMs without the ability to explain them, society will enter this new era of AI blindfolded, without robust tools for anticipating, auditing, or regulating the mechanisms of these large-scale systems, even as they begin to impact every aspect of society.

A national deep inference research computing facility for LLMs is necessary due to the unique computational needs of large-model inference research. Performing LLM inference consumes quadrillions of parallel computations in a fraction of a second, requiring both (1) high-performance parallel GPU computing capacity, beyond the scale that is feasible at an institutional level, and (2) software infrastructure to enable scientists to share those high-capacity computing nodes for very brief experiments. Neither existing HPC clusters nor commercial inference services address these needs. HPC clusters do not scale to thousands of simultaneous inference users; and commercial inference services hide internals of the LLMs (Figure 1a), making them unsuitable for research. **The National Deep Inference Facility (NDIF) will enable scientific interrogation of LLM mechanisms by providing a unique scalable transparent deep inference service (Figure 1b), harnessing the high-performance GPU capacity of the NSF DeltaAI project (Figure 1c) to advance urgently needed understanding of *how* LLMs work so industry, government, researchers and the public are able to safely deploy, regulate, use, and study them for the benefit of society.**

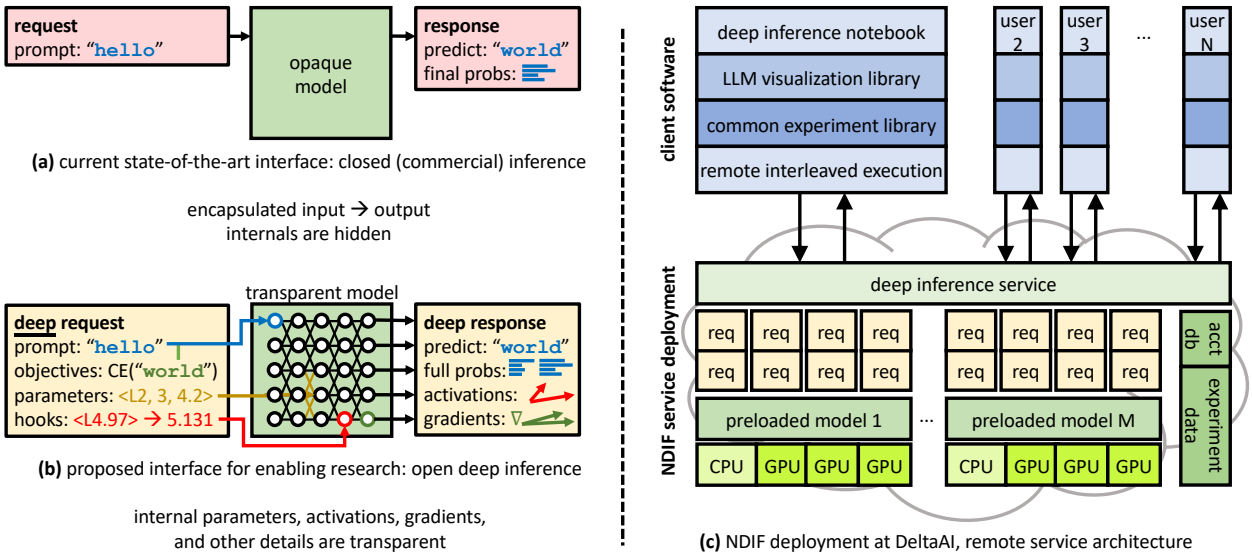


Figure 1: (a) Current services hosting large language models provide very limited interaction functionality (Top). One can send input text in a request, and is then provided an output string (and in some cases scores for predictions). (b) We propose developing infrastructure to provide deep access *to hosted language model instances (bottom), which will permit critical research without necessitating researchers hosting such models themselves. (c) The infrastructure consists of new software libraries and a deployed distributed service to be shared by researchers nationwide.*

NDIF will run on the NSF-supported NCSA DeltaAI project, a recently-funded AI-focused computing resource that consists of a large and uniform pool of compute nodes that provide the high-memory GPU configurations that are necessary for the highly-parameterized massively parallel computations of LLM research. By "deep inference" we mean the instrumentation and study of the behavior, mechanisms, and impact of an AI model when it is used to perform tasks *after* it has been trained. NDIF consists of three complementary components:

1. Creation and deployment of an online **inference service** hosted at the NSF-supported NCSA DeltaAI cluster, allowing researchers to interrogate and conduct ground-breaking research on the largest available and most scientifically relevant LLMs. (Figure 1c).
2. Development of **open-source server and client software** that will power the service, enabling convenient, transparent and scalable remote execution of experiment protocols by a broad community of researchers, efficiently sharing large models at the online inference service.
3. **Outreach and training** for students and researchers in every region of the country to use NDIF to advance understanding of large neural network models, developing a highly skilled workforce of scientists and engineers to lead the world in ethical use of state-of-the-art LLMs.

NDIF will be developed under the leadership of a unique team of experts in machine learning, software engineering, deep network interpretability, language modeling, and inclusive computing at Northeastern University (NU). The team will benefit from the university's well-established organizational structure and advanced facilities. The deployment of the service will be done in close collaboration with the DeltaAI project at National Center for Supercomputing Applications (NCSA) at University of Illinois Urbana-Champaign, who will provision and host the computational resources (see attached letter of collaboration from DeltaAI).

2 Intellectual Merit

Explaining AI systems is a national and global priority: In October 2022, the White House Office of Science and Technology Policy released a Blueprint for an AI Bill of Rights [8] delineating a consumer's right to AI systems that "*provide explanations that are technically valid, meaningful and useful.*" In January, 2023, the National AI Research Resource Task Force [10] identified one of the four critical opportunities for strengthening the U.S. AI R&D ecosystem as the development of trustworthy AI by ''*supporting research on AI's societal implications, developing testing and evaluation approaches, improving auditing capabilities, and developing best practices for responsible AI R&D can help improve understanding and yield tools to manage AI risks*." In March 2023, the Future of Life Institute published a "Pause Giant AI" open letter [9] which has since garnered more than 25,000 signatories, including many national leaders in AI research, recommending "*a significant increase in public funding for technical AI safety research in the areas of alignment, robustness and assurance, and explainability and interpretability*" [11]. These three documents (from diverse prospectives) highlight the shared urgency for research to explain, audit, evaluate, and manage impacts of large-scale AI.

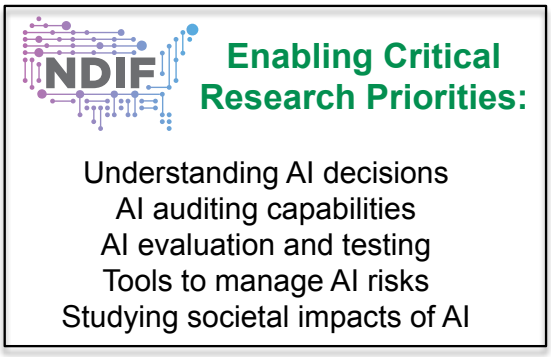
Meanwhile, **LLMs such as ChatGPT are being adopted more quickly than any previous technology**, with widespread deployment in consumer-facing technologies [12–14], touching every field involving reading, writing, or programming, even as its mechanisms remain unexplained [2, 15]. Because we do not understand how LLMs make their predictions, we find ourselves in a situation where the most impactful class of AI model today is inscrutable: the **opacity of LLMs has become a foundational challenge to our national goal of developing trustworthy AI**. Academic researchers are ideally-suited to investigate the mechanisms of LLMs, but are unable to conduct this critical research due to the lack of large-scale LLM research infrastructure – a new need that stems from from the unprecedented scale of state-of-the-art LLMs.

Deep inference has unique computational demands. The computing required to support research into LLM inference is not well-supported by either traditional HPC provisioning nor existing

commercial inference services. Commercial inference services provide no access to model internals and are therefore unsuited to scientific research. HPC batch allocations, which could provide full access, partition computational resources among users by giving a user exclusive use of capacity for a period of time. This precludes thousands of researchers from performing concurrent experiments on the same models on shared computers. NDIF will solve these critical needs by aggregating together many different researchers' requests to efficiently use existing HPC resources at DeltaAI. Unlike commercial inference services, NDIF will have a unique design, informed by the community of LLM researchers, that will provide the ability to perform inference together with experimental code that can inspect, analyze, and modify every aspect of LLM computations (Figure 2), enabling a wide range of scientific research.

2.1 Scientific justification

The unique LLM deep inference capabilities provided by NDIF will enable scientists to advance **five critical research priorities identified by the NAIRR Task Force** [10], specifically enabling scientists to advance a) understanding of AI decisions; b) AI auditing capabilities; c) AI testing and evaluation; d) tools to manage AI risks, and e) research on societal implications of AI.



a: Improving understanding of AI decisions. Mechanistic understanding of LLMs could transform how such models are used, developed, and regulated. Explaining LLMs is challenging because they are massive artificial neural networks, i.e., computational systems loosely inspired by human neurons [16, 17], with connection strengths determined by an data-driven training process [18, 19]. Because LLMs are not programmed explicitly, the only path to an explicit understanding of their calculations is reverse-engineering their internal computations, which is challenging due to their complexity. The scientist community involved in NDIF design includes experts on methods for understanding both artificial [20, 21] and biological [22] neural networks, part of a growing community investigating the inner-workings of LLMs (e.g., the BlackboxNLP workshop [23]). We have worked with this community to identify capabilities of the NDIF that would empower work on cutting-edge experimental methods, as discussed in Section 2.2.

b: Improving AI auditing capabilities. Auditing LLMs would allow users to identify the knowledge contained within a network. This capability could be transformative by redefining the way that humans interact with LLMs, potentially revealing the degree to which models encode bias [24, 25], sentiment [26], linguistic knowledge [27–29], truthfulness [30, 31], and many other kinds of information [32–34]. By providing the unique capability to apply representation analysis to LLM internal states, NDIF will allow scientists to extend auditing capabilities for modern LLMs.

c: Developing AI evaluation and testing methods. Rigorous evaluation of LLMs is essential, especially when they are applied in high-stakes application areas such as bio-medicine [35]. For example, high-stakes settings raise critical evaluation issues in applications such as detecing dementia [36], measuring fairness [37, 38], and studying risks of potentially sensitive personal health training data [39]. Many of our community members are performing such research with opaque model access to GPT-3/4, where they do not have complete control over the evaluation setting. In contrast, NDIF will provide capabilities needed for rigorous evaluation, including complete access to output probabilities, internals, and the ability to fine-tune and evaluate models transparently.

d: Creating tools to improve AI safety and manage AI risks. NDIF will enable the development of tools that could be used to mitigate the negative impacts of LLMs, enabling research into

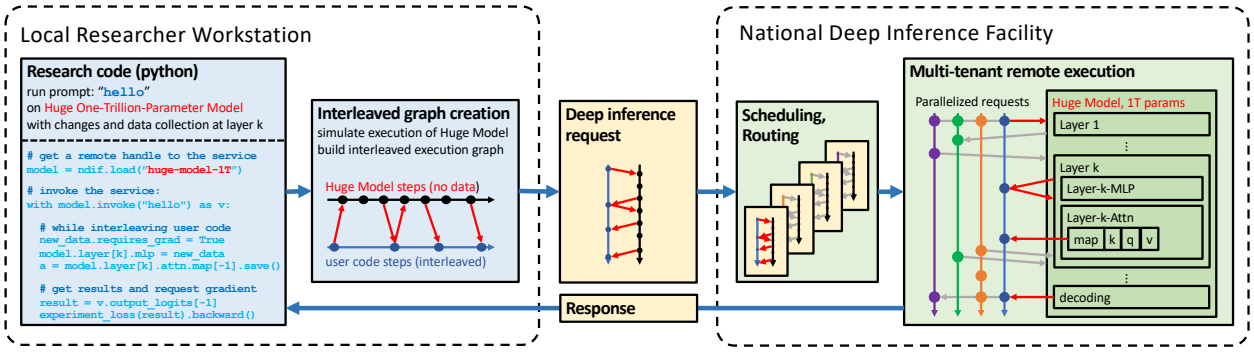


Figure 2: Details of the logical view of a deep inference request. Unlike commercial inference that provides no transparency, the NDIF will allow researchers to execute flexible experiments by interleaving their own code within the internals of the deep network inference process. To maintain safe and efficient co-tenancy, experiments are submitted as computation graphs that enable resource accounting and scheduling.

both short-term risks and long-term risks posed by very large AI models. NDIF will enable research into the detection of machine-generated misinformation [40–42], tools that could detect and mitigate untruths or deception in a model's behavior [30, 31, 43], and methods to erase undesired behavior [44] or improve stability of behavior over long time horizons [45]. Such research requires full access to posteriors and activations, as uniquely provided by NDIF.

e: Enabling research on societal impacts. Understanding social impacts requires studying interactions between LLMs and people. For example, our users include social scientists interested in how people behave differently when talking to a chatbot, and in how persuasive LLMs are. Already, LLMs have been used to judge public opinion [46], to measure political ideology and latent constructs [47], and to analyze text as data [48]. But social scientists tell us that commercial APIs do not provide the transparency that would allow reproducible research. NDIF will provide an environment for ethical human subjects research and will provide both the technical capabilities to support human studies and a process to allow protocols to be overseen by a researcher's IRB.

2.2 Experimental methods uniquely enabled by the NDIF service model

To enable scientists to advance the research agenda in Section 2.1, NDIF will enable a wide range of experimental methods in a **flexible unified framework, allowing researchers to interleave their own experiment code in large models hosted remotely**. This will allow researchers to gather and analyze every aspect of the neural network's internal data (Figure 2). The unified framework will enable critical technical experimental methods that are unavailable via commercial LLM inference services, including *representation probing* [32] and other forms of *representation engineering* [49] such as *causal alignment mapping* [50, 51], *sparse dictionary learning* [52–54], other trained probes of semantics and structure [55–57], and individual neuron studies [26, 58–61]. NDIF will also support *salience mapping* via *gradient methods* [62, 63], as well as access to *attention distributions* [64–66] and *per-token probabilities* [67]. Access to activations will also enable neuroscience-inspired methods such as *representational similarity analysis* [68, 69] and *latent factor analysis* [70–72].

The same framework will also allow direct counterfactual interventions into model internals, which will also enable *causal mediation analysis* at the level of individual neurons [73, 74], representation vectors [75, 76], or subspaces [50, 51]; these methods will also enable *circuit-finding methods* [77] such as *path patching* and *activation patching* [78–80]. The service will also support gradient-based optimization of inserted parameters, to enable *parameter-efficient fine-tuning* (PEFT), which will enable investigations into the intriguing transfer-learning capabilities of LLMs through *soft prompts* and *adapter layers* [81–83]. The same optimization support will also be a tool for creating representation probes [32] and for other training-based experimental methods [50–52, 54].

2.3 NDIF will leverage all existing and future open LLMs

Efforts to train open LLMs are complementary to NDIF, as NDIF focuses on addressing barriers to research at the *inference* stage on those open LLMs, after they are trained. NDIF will integrate with every pretrained model that makes its parameters available to academic researchers, adding specialized support for the most popular models. We will collaborate and support ongoing efforts to encourage and deploy new large open models. We will integrate with: (1) **EleutherAI GPT-NeoX** [84], **GPT-J** [85], and **Pythia** [86], 6-to-20 billion parameter LLMs with fully reproducible training data, trained by the EleutherAI nonprofit. (2) **Meta OPT** [87], **Llama** [88], and **Llama 2** [89], sets of models up to 65-to-175-billion parameters trained and licensed by Meta, with parameters available to academic researchers. (3) **AI2 OLMo**, a 70-billion parameter family of multimodal models trained by the Allen Institute for AI planned for 2024. (4) **BigScience Bloom** [90], a 176-billion parameter multilingual model trained by BigScience, a collaboration of European agencies. (5) Model variants fine-tuned with for conversation or multimodal use, including BigScience Bloomz [91], CarperAI [92], Alpaca [93], Vicuna [94], and OpenFlamingo [95]. (6) Ongoing work by the National AI Research Resource (NAIRR) [10], LAION [96], MosaicML [97], and Together [98]. We anticipate many additional publicly available LLMs each year; our configuration committee and scientific advisory board will prioritize model support for maximum scientific impact.

3 Research Infrastucture Development

3.1 Technical readiness

Our team has created a detailed Project Execution Plan (PEP) that delineates requirements, design, and deployment milestones for the NDIF's user model, user-facing and internal software, training, and outreach. We have created a prototype implementation that includes the core interleaved execution framework that will allow the NDIF to efficiently support a wide range of research methods, and we have created an set of online tutorials that demonstrate use of NDIF to reproduce recent scientific results. Testing is underway with the prototype in use by five pilot users conducting research with the system. Please see our attached PEP and Technical Platform Specification for complete details on the development schedule, project management plan, and system design.

3.2 Major deployment milestones

Development and deployment of NDIF will proceed in several phases, each one increasing NDIF capabilities, robustness, and usability. The plan is designed to deliver value to researchers as early as possible while maximizing opportunities to respond to user feedback and outside events.

Closed pilot, Q1 2025. In the first phase, we will create a web API that can support interleaved-execution research queries observing and intervening in inference for the largest models with open parameters (70b-175b parameters), with both streaming and batch-oriented use patterns, supporting all forward-pass experimental methods. The goal of the project at this stage is to develop the system while validating the system design and user model with a small set of early adopters drawn from our design-participant user community. These early users will work directly with our team and will provide direct design feedback. The team will produce documentation, tooling, and support sufficient to meet pilot user needs. The pilot will culminate with a usage demonstration to teach 100 users to use the system at a major conference tutorial session. Hardware needs: 2 CPU servers and 10 4x A40 GPU nodes, which are already currently deployed at NCSA.

Nationwide open pilot, Q1 2026 (Year 2). In the second phase, we will make the service available openly for early access to all qualified users at any educational institution. Achieving broad usage will require us to provide a stable service with increased robustness, including monitoring and alerting systems, job queuing, and a fairness-oriented scheduler. In this phase we will define Service Level Objectives (SLOs) and measure progress toward meeting them. We will expand functionality to include backpropagation experimental methods and deploy reproducible fine-

tuning and optimization functionality. The API will be stable and documented well enough for online self-service, and we will flesh out online tutorials demonstrating all major research methods. We will teach usage of the service at a large local workshop, and demonstrate the service at a large conference tutorial. Hardware capacity needs in year 2 and beyond will be driven by demand; we estimate 4 CPU servers and 10 4x A40 GPU nodes, currently existing, plus 5 4x H100 nodes for large models, growing to 10-20 4x H100 nodes, to be provisioned from DeltaAI based on demand.

National outreach bootcamp and software API full release, Q1 2027 (Year 3). The third phase is concentrated on broadening usage, which will require a high degree of stability, learnability, and functionality. All major user-facing features of the system will meet SLOs, which will require development of refined monitoring and administrative tooling. Support will be added for dedicated allocation for heavy users, to reduce contention on the public queue. User-facing documentation must be complete and tested, and virtual and in-person bootcamp curriculum will be developed and delivered. Over 300 researchers from diverse institutions will be recruited and taught to use the system in a multi-site bootcamp. Capacity in years 3 and beyond will be planned in close coordination with the NSF and NCSA, based on an assessment of community needs.

Operations scale-up, Q1 2028 (Year 4). The fourth phase focuses on scaling the system to support new and larger models to match the state-of-the-art. At this stage, the NDIF will be pivotal in enabling new research on the largest models: its availability should encourage the training of larger-scale academic models, since NDIF will allow researchers to routinely be able to study and reproduce large experiments. We also will continue to expand capacity to meet demand from new users, and we will measure and refine the user experience to improve our ability to efficiently onboard and support new users. We will improve system administration tools to improve issue response and provide a high level of stability. And we will pilot ability to run NDIF workloads on other clusters, to provide a higher level of availability than can be achieved in a single cluster.

4 Metrics and Annual Goals

We will continuously monitor metrics to track the progress of the NDIF project, including (1) Users by amount and diversity (2) Training, outreach, and educational programs delivered (3) Specific research capabilities deployed. The purpose of NDIF is to broadly enable LLM research to enable transformative science and workforce development; therefore the primary goal each year is to enlarge and broaden usage, and to expand research capabilities and outreach to enable that goal. Table 1 summarises high-level goals per-year.

We also summarise the major capability goals for the platform each year. *Year 1:* all major forward-pass inference and intervention methods supported on all open models up to 175 billion parameters. *Year 2:* Parameter-efficient fine-tuning and optimization. Usage accounting and fairness-oriented scheduling. *Year 3:* Support users with heavy usage patterns through approved allocation process. 90% or better continuous uptime, and a set of SLOs are defined, monitored, and met. *Year 4:* Capacity meets current state-of-the-art models and user demand. 90% or better

Metric		Year 1	Year 2	Year 3	Year 4
Users	Active per-month	20	100	1,000	2,000
	States represented	3	20	30	50
Training	Conference tutorial attendees	50	100	100	100
	Week-long bootcamp attendees		100	300, multi-city	100
	Online curriculum	Prototype	Deployed	Revised	Revised

Table 1: Annual goals for high-level metrics. This is a non-exhaustive list of metrics that we will track, review and report. Section 3.9 of the PEP provides a detailed breakdown of milestones.

continuous uptime, and other SLOs are met. The availability of NDIF has enabled major research findings and should be cited in motivation of release of 10^{13}-scale models for academic study.

In addition to the above metrics and goals, throughout the project we we will monitor user diversity, research citations, user feedback, issue response, feature usage, system performance, and system availability. Section 9.11 details our overall project evaluation process.

5 Coordinated Scale-out with NCSA Delta and DeltaAI

We will develop and deploy NDIF utilizing HPC resources operated by the DeltaAI project at the National Center for Supercomputing Applications (NCSA), and we will coordinate deployment with them via biweekly meetings (see the attached letter of collaboration from NCSA director William Gropp). DeltaAI is building computing capacity that is well-suited to NDIF. Together we have estimated an appropriate allocation to this project as part of our proposal. Our initial capacity needs for the first year (estimate: 2 CPU servers and 10 4x A40 GPU nodes) are already available through the Delta cluster. By year 2, we expect to need larger GPU nodes (5-20 4xH100 nodes), which will be built as part of the recent NSF DeltaAI award. We will scale capacity up and down as needed to support demand. For capacity in years 3 and beyond, we will assess demand and current state-of-the-science and discuss with the NSF how best to meet needs of the community, including whether there is a need for additional nodes in DeltaAI or in the NCSA storage environment (for example higher-VRAM nodes or next-generation interconnects). Initial development resources will be allocated through the ACCESS program, and we will work closely with the NSF and NCSA to determine the appropriate allocation method for the service in deployment. Computational capacity will be provided by DeltaAI and is not included in the budget for this project. Each quarter we will track and report utilization metrics to support discussions with DeltaAI and the NSF on how best to meet computational capacity needs of the research community.

6 Outreach, Training and Dissemination Plan

The NDIF will strengthen the US Artificial Intelligence Research & Development ecosystem by providing training and support to the US scientific community to ensure that the infrastructure is accessible and usable, and to address knowledge, technical, and social barriers that could limit adoption. Core to our outreach plan is an effort to build a scalable network of experts who can respond to local needs. Our training, outreach, and dissemination plan consists of the following:

Nationwide online curriculum We will design training modules to help onboard new researchers and students to NDIF. Modules will cover topics such as: 1. Understanding large foundation models. How to visualize and understand their internal operation using NDIF. 2. How to apply deep inference methodologies such as representation analysis, salience mapping, causal mediation analysis, circuit analysis, and parameter-efficient fine tuning. How to use NDIF to apply these analysis methods. 3. Recent scientific results on auditing, evaluating, and controlling behavior of LLMs with respect to interpretability, bias, safety, robustness, or other task performance. How to reproduce recent research results and extend experimental methods using NDIF.

NDIF week-long bootcamp workshops (Years 2, 3, 4) We will develop and deliver an intensive week-long bootcamp workshop program which will provide graduate students studying in the U.S. with a rapid survey of cutting-edge LLM methods, taking advantage of NDIF infrastrcuture. The purpose of the workshop will be to quickly upskill participants in LLM research methods, taking advantage of NDIF infrastructure. The workshop will begin with LLM fundamentals and culminate with coverage of current research results in LLM interpretability, evaluation, control, and applications. In years two and four, the workshop will be held in Boston, hosting 100 students. In year three, we will conduct a multi-city bootcamp series to reach over 300 students in six geographic regions, leveraging NU's campus network and two university partners, in Oakland, Miami, Washington DC, Dallas, Chicago, and Maine. The cost of attending the bootcamp will be

free (leveraging the NU campus network) and will be led primarily by Northeastern PhD students with co-PI Bell and co-PI Guha in attendance. For graduate students whose advisors do not have budget to cover the travel costs we have budgeted a $150k fund to support travel based on need and impact; in awarding these we will prioritize EPSCoR states, MSIs, and PUCs.

Machine learning conference tutorial series We will also offer one-day workshops using the in-person tutorials co-organized with major machine learning conferences (e.g., NeurIPS, ICML, ICLR, ACL, EMNLP, AAAI). We will select one conference each year with the goal of maximizing the diversity of locations in the U.S. The students who participate in the bootcamps and tutorials will become part of a network of experts, providing embedded expertise within their own institutions, and helping us to provide support that is responsive to local needs across the nation.

Undergraduate education We are committed to ensuring that undergraduates in the U.S. benefit from NDIF. To this end we will develop materials—lectures, exercises, and assignments—that cover analysis of large language models. We will pilot and refine these materials in relevant courses at NU (e.g., Machine Learning I and II, NLP, and Neural Networks). PI Bau and Co-PI Wallace regularly lead these offerings. Further, Wallace is Director of the Bachelors in Data Science program (and serves on the undergraduate curriculum committee), so is well-positioned to ensure that developed materials are incorporated into course curricula. Once developed, we will make materials—which will use the hosted NDIF API—publicly available and we will support their use by to faculty at other institutions, scaling the impact by enabling U.S. undergraduates in CS to gain hands-on experience analyzing and working with the internals of LLMs. This is not currently possible at the vast majority of institutions given the resources required to run such models (and the limited access to model internals that commercial APIs provide). We will ensure that we support universities and colleges across the country with a particular focus on outreach to EPSCoR jurisdictions and a diversity of institutions, including SLACs and MSIs.

Democratic and equitable outreach It is critical that we ensure that the NDIF does not further widen the gap between AI researchers from majority groups and those from groups historically marginalized in tech [99, 100]. Thus throughout all outreach we will ensure that we are reaching a diverse set of institutions, researchers and students, with a focus on reaching early-career faculty, and professors in EPSCOR states, MSIs, PUIs, and CCs. Co-PI Brodley, who is a nationally recognized expert in broadening participation in computing [101], will lead this effort. We will recruit potential using popular social media channels such as X, through the CRA (see attached letter from CRA Exec Director Tracy Camp), by running workshops at AI/ML conferences, and by utilizing the deep network of 100+ (R1 and non-R1) institutions that already participate in initiatives run by the Center for Inclusive Computing (led by co-PI Brodley).

7 User Engagement and Open-Source Community

Support for the NDIF project is strong in the US research community — **over 400 researchers indicated that their research goals were blocked in a twitter community survey.**

Many emphasized the strong need for infrastructure given the practical difficulties of investigating models whose parameters do not fit into the memory of typical research computing nodes. Professor Boaz Barak (Harvard) observed, "Any model that doesn't fit on one GPU starts to be complicated for researchers to use even if they do have enough GPUs to fit... A central engineering resource that all academics can share would be a game changer." Professor Tom Dietterich (Oregon State) said, "I strongly support a public National Deep Inference service.... We will want to support many different things: fine tuning, access to the training data, access to external resources." Professor Zoltan Majdik (North Dakota State) laid out the benefits: "Interpretability would easily be my number-one target. On multiple levels: for academic LLM experts, but also ... make interpretability interpretable for social scientists, non-computer-science." Professor Ana Marasović (University

of Utah) noted, "Having academic access ... would enable not only machine learning academics, but also academics without expertise in training models, to study large language models."

7.1 Gathering user requirements through virtual and open-source communities

Based on strong and broad interest, we have established a virtual research user community (NDIF-VC) that includes 40 professors from 34 different universities in 19 states including 5 EPSCoR jurisdictions (see Figure 3), and 8 minority-serving institutions (including an HBCU) who have suggested specific research projects that will benefit from NDIF. The researchers, who will directly use NDIF as early adopters, span a broad range of disciplines both inside and outside computer science. Their discussions have informed the required research capabilities (Section 2.2) and design of NDIF.

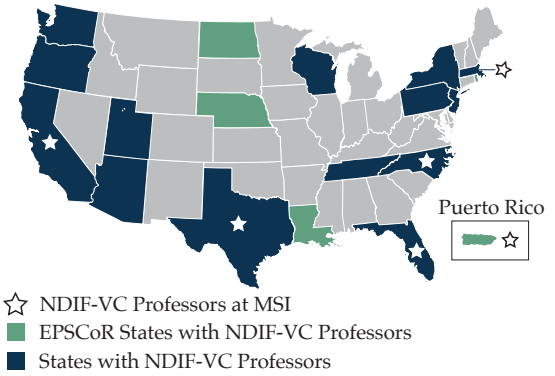


Figure 3: National reach: Our existing virtual community (VC) includes faculty at 34 universities in 19 states (5 EPSCoR jurisdictions) who have proposed specific research to be done with NDIF.

To support this virtual community, we maintain a *Discord* server, bringing together researchers from across the country for both asynchronous and real-time discussions. We also maintain a website with reference materials, tutorials, and examples [102], and share the open-source codebase on GitHub with full code and technical specifications. As NDIF is deployed, we will welcome participants into this community and organize an Annual NDIF Virtual Conference, providing students and researchers with a space to showcase their ongoing work and to have "ask me anything" interactions with the project team.

We will use the GitHub public issues tool as well as the Discord virtual community to gather, track, and discuss user issues. The open source committee will meet quarterly to review, identify and summarize themes from the virtual and open-source community, and these findings will be reported to NDIF leadership to help inform the technical and policy direction of NDIF.

8 NDIF User Access

The research community will access NDIF in several ways, described below:

NDIF website usage The NDIF service will offer a web interface open to any person with an educational affiliation to use free-of-charge (using the NSF and DOE-supported "CILogon" Service for authentication), after agreeing to a service agreement and submitting a brief statement of intended use. Once a user is enrolled, they will have access to a code-free web interface that allows direct chat-style interactions with large models, and that also enables *Logit Lens* visualzations [103–105] of language model internal states during inference.

NDIF API usage Most users of NDIF will use NDIF through the API and python client library. After establishing an account on the website, users can get an API key that can be used together with the NDIF python library, that allows them to write code that performs deep inference on NDIF-hosted models remotely. The library is more flexible and powerful than the web interface alone, because it provides an interleaved-execution context (Figure 2) that allows a researcher to interleave custom experiment code between the steps of a large model, providing full access to model internals and interventions, with a concise and highly reproducible idiom. Programmatic requests can be submitted and fulfilled either serially in best-effort-real-time, or queued in batches of requests whose results are returned asynchronously.

Local API usage The client library will be open source and available to be used freely by all without an NDIF account. As illustrated in Figure 4, the library can be used for local experiments on any pytorch model; it will enable interleaved local model experiments using the same idioms

used for huge models hosted by NDIF. The purpose of this design is to provide a smooth "on ramp" where students and researchers can learn and develop their ideas locally, and then use exactly the same code to conduct huge remote model experiments. Since the client library is designed to improve researcher quality-of-life even for small experiments, we aim for and expect broad usage of the library even in client-only mode.

High-volume usage To support high-volume use and to efficiently utilize underlying DeltaAI resources in both high- and low-load conditions, NDIF will design and implement a provisioning technology in collaboration with TAPIS open-source ecosystem, autoscaling Kubernetes containers on Slurm. This will integrate with ACCESS provisioning to accommodate approved users with heavy usage patterns. We will design this system in collaboration with the TAPIS team, meeting with them regularly to consult on the usage of TAPIS in our application. (See letter of collaboration from Joe Stubbs, Development Manager of TAPIS.)

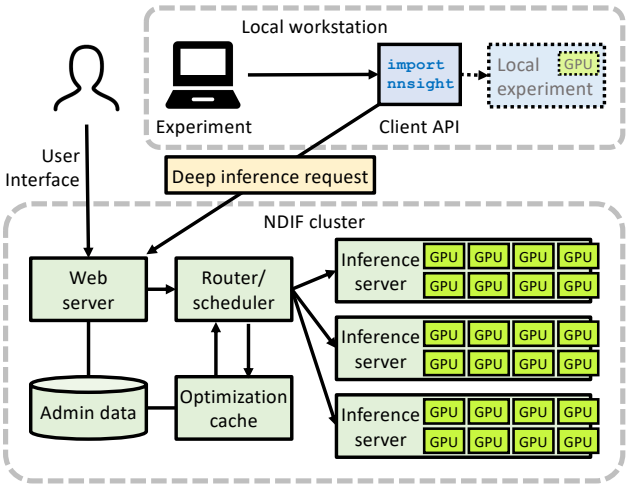


Figure 4: NDIF service architecture, showing request flows between system components.

9 Project Management, Operations and Utilization

9.1 Key Personnel

Figure 5 shows the organization chart. This project brings together an interdisciplinary group with deep expertise in ML/NLP, programming languages, software engineering, and large-scale computing, as well as experience in development and operation of large-scale computing systems and the creation and administration of multi-institution research programs.

PI Bau - NDIF Director (Assistant Professor, Khoury College of Computer Sciences, NU) brings a unique skillset as a late-career academic who worked in industry for 20+ years, 12 of them at Google. There, he created and managed the Google Talk team and led Boston Google Image Search ranking. He has the track record to implement an infrastructure of this scale, having successfully managed projects to develop large-scale online platforms with global reach and real-world impact, processing exabytes of data and answering billions of user queries. Since transitioning to academia, PI Bau has established himself as a leading researcher in interpretability of large neural networks [58, 106–108] and model editing [44, 109–112], and he has been a pioneer in the characterization of causal mechanisms within LLMs [34, 75, 76, 105, 113, 114]. As NDIF Director, Bau will hire and manage project leadership and oversee the overall success of the facility. He will work closely with the project manager and lead software engineer to manage the project and will run monthly meetings of NDIF leadership. He will also serve on the technical configuration committee.

Outreach Lead and Co-PI Brodley (Dean of Inclusive Computing, Founding Executive Director of the Center for Inclusive Computing, NU; former Dean of Khoury College) is a fellow of the Association for Computing Machinery (ACM), the Association for the Advancement of Artificial Intelligence (AAAI) and the American Association for the Advancement of Science (AAAS). Her interdisciplinary ML research has advanced computer science as well as remote sensing, neuroscience, digital libraries, astrophysics, image retrieval, computational biology, chemistry, and evidence-based medicine. Brodley will lead outreach efforts (WBS 1.3) and ensure broad participation in setting research priorities and the educational mission of NDIF. She will chair the outreach and training committee. She will serve as liaison to the public interest technology

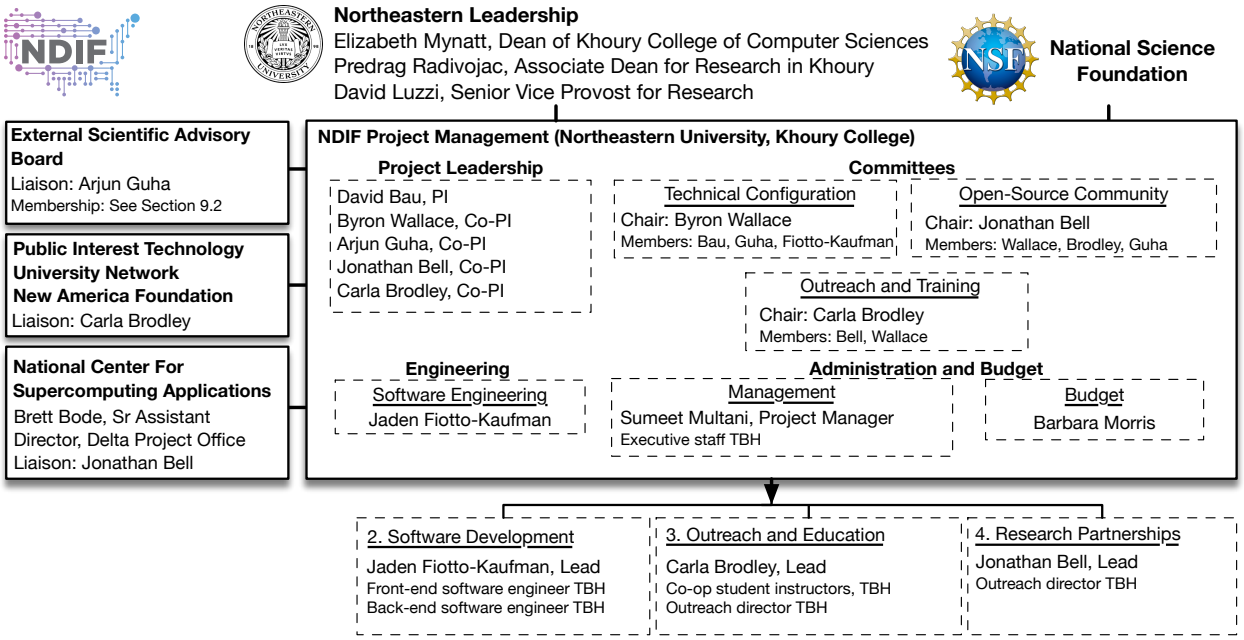


Figure 5: NDIF organization

university network, and will serve on the open-source community committee.

Co-PI Wallace - Technical Configuration Committee Chair (Sy and Laurie Sternberg Interdisciplinary Associate Professor in Khoury College of Computer Sciences, NU) has extensive research expertise in NLP and interpretability of such models [115–122], as well as their use in biomedical settings [39, 117, 123–125]. Wallace will chair the Technical Configuration Committee, which will meet at least quarterly to review the design of the service and ensure that its design meets research aims. Wallace will be responsible for establishing academic priorities for the facility, and for conducting outreach to the NLP and biomedical research communities. He will serve on the Open-Source Community Committee and the Outreach and Training Committee.

External Advisory Board Liaison and Co-PI Guha (Associate Professor in Khoury College of Computer Sciences, NU) brings deep experience in programming languages, including language-based security [126–129], GPU accelerated domain specific languages [130, 131], and pre-trained models for code generation [132]. Guha will serve as liaison for the External Scientific Advisory board and will be responsible for engaging and recruiting leaders of the academic community to the board to ensure that long-term needs of the academic community are met. Guha will also serve on the Technical Configuration Committee and the Open-Source Community Committee.

Open-Source Chair and Delta AI Liason, Co-PI Bell (Assistant Professor in Khoury College of Computer Sciences, NU) is an expert in software engineering and systems, including architectural design [133], testing and continuous integration [134–137], and analysis [138–140]. As chair of the Open-Source Community Committee, Bell will be responsible for incubating the open-source community and overseeing open-source activities, providing academic oversight on open source policies, technical contributions, and quality assurance. Bell will also serve as liaison to the Delta AI project, ensuring coordination and communication with that team with respect to technical design and capacity. He will also serve on the Outreach and Training Committee.

Project Manager, Multani has extensive experience leading the definition, planning, and execution of both user-facing and infrastructure projects and has served as a technical program manager at Google, TripAdvisor, and Akamai Technology. As project manager, Multani will work closely

with the PI, and all work areas of the project (WBS 1.1-1.4). He will be responsible for management of schedule, budget, scope, and risk. Additionally he will be responsible for all NSF reporting, including quarterly reports, annual reports, and periodic PEP updates.

Lead Software Engineer, Fiotto-Kaufman has spearheaded the technical design and prototype for NDIF. Previously, he served as research scientist and led a wide range of research engineering projects in machine learning and artificial intelligence at Raytheon BBN. As lead engineer, he will be responsible for hiring staff engineers, and for managing the development process (WBS 1.2). He will serve on the Technical Configuration Committee.

9.2 External Scientific Advisory Board

We will establish an External Scientific Advisory Board to provide input into key aspects of the project. The board will consist of 5-10 members, each of whom will be a subject area or project management expert or representative of a relevant constituency such as a university administrator. One member of the board will represent the Delta AI project. Several prominent members of our academic user community have offered to serve as initial board members. The advisory board will meet twice per year, once virtually and once in person.

9.3 Scope control

The Technical Configuration Committee and the PIs will define the experimental capabilities that will be enabled by NDIF during each phase of deployment. These decisions will be made in consultation with the External Scientific Advisory Board and open source community. Agile project mangement methods will be adopted to continuously test the product to iteratively identify and solve problems and to improve the software. The Technical Configuration Committee will conduct an annual review to identify changes in scope and determine where corrections are needed.

9.4 Delta AI / NDIF coordination meeting

The NDIF and Delta AI teams will meet regularly on a biweekly basis, to coordinate technical design and operational and capacity planning. The goal of this meeting will be to coordinate on hardware and cluster configuration and allocation decisions, and also to establish channels of communication for and planning outages and for responding to issues.

9.5 Engaging the public-interest technology research community

The benefits of advances in AI have been realized unequally [141]. To ensure that NDIF enables critical assessment of the potential impact of LLMs on education, policy, privacy, and safety we will work with the New America Foundation's Public Interest Technology University Network (PIT-UN) to bring both AI and non-AI faculty to workshops with AI researchers/students to discuss issues of interest and promote the public good (see attached letter of collaboration). PIT-UN has a membership of 63 universities and colleges, 19 of which are Minority Serving Institutions (MSIs). PIT-UN will support NDIF by establishing a Public Interest Technology (PIT) Advisory Group comprised of 10-15 interdisciplinary experts from both technical and social sciences, to provide guidance on the responsible and ethical design, development, deployment, and use of LLMs.

By undertaking the LLM project, PIT-UN aims to meet the following goals: (1) Engage conversations regarding LLMs to be community-driven; (2) Promote equitable and broad participation in the emerging field of AI through LLMs; (3) Advance the knowledge base of LLM learning by advancing PIT with formal reports out from New America reflecting feedback from semi-annual roundtables of its Advisory Group; (4) Develop formal learning experiences and environments through strategic activities in collaboration with other New America teams such as Open Technology Institute and the Ranking Digital Rights program as needed to support and represent possible frameworks; (5) Develop professional capacity within member universities themselves to deliver informal AI learning using the LLMs within a PIT framework; (6) Host an annual webinar to distill key findings and build a base of new AI learners through exposure to PIT and its applications

related to LLMs.

9.6 Budget and budget contingency

We begin with a baseline budget and budget justification included with this proposal. Throughout each phase of the project, the project manager will update the budget and provide NSF with updated cost estimate for both capital and soft costs. We set $450,000 (5% of total budget) as the budget contingency, which covers any extra costs, including risk, increases in scope, and unknown tasks. This money is not allocated to any area of work and will only be used as needed.

9.6.1 Schedule and schedule contigency

The proposed effort will run from 4/1/2024 to 3/31/2028; please find the schedule in the PEP. In each year of the project we schedule a single major deployment release. Uniformly throghout the schedule, we set aside 5% schedule contingency, to allow time for unanticipated integration, quality assurance, or adjustments in scope. In that case, the project manager will conduct a review to adjust scope, timing, and budget of the project.

9.7 Risk management

Risk Identification. We will identify project risk through structured brainstorming sessions with stakeholders through the duration of the project, utilizing SWOT analysis, cause and effect diagramming, assumptions analysis, and risk breakdown structures. The project manager will conduct sessions focused on risk categories, e.g., scope risks, financial risks, and quality risks.

Risk Analysis. The project manager will analyze risks identified through structured brainstorming sessions using a variety of qualitative and quantitative methods, including SWIFT analysis, interviewing experts, analysis of expected monetary value, and sensitivity analysis. This analysis will be used to establish the appropriate risk tracking and control procedures.

Risk Tracking, Control, and Monitoring. The risk-mitigation process will guide us in selecting appropriate mitigation strategies for each risk, given the value impact and probability of each option. Risk will be tracked over time, and the effectiveness of the risk-management process will be tracked. Project leadership (the PIs, project management, and lead software engineer) will conduct a comprehensive review of risks annually, reviewing each risk to develop mitigation strategies. As the project proceeds, each risk will remain on the risk register until it is closed. We have conducted an initial risk assessment (refer to the PEP for the risk register). Some of the major risks include hardware failure, user adoption risk, and software technical performance risk. Our project plan mitigates these risks where possible.

9.8 Configuration Management

Changes for all project specifications other than software, such as specification of required infrastructure capabilities or changes in policies or legal agreements, will be managed through a formal change control process. Staff and leadership will propose changes with input from external stakeholders, and the changes will be reviewed by the Technical Configuration Committee. Updates to specifications will be communicated at the required time, for example during contract renewal. Change control for software will be narrowly controlled by the software engineering team, utilizing software version control through git. Changes will go through code review and will be unit tested before being committed. Integration tests will be conducted before deployments, and deployment version numbers and a change log will be maintained.

9.9 Operations management and governance

After successful deployment of NDIF, the facility will transition to ongoing operations, with the goal of maintaining the service infrastructure to ensure its continued availability to the research community. In the operations phase, NDIF will retain its facility director and external advisory board, and an operating staff that will conduct training, support, and issue management.

9.10 Operating costs and funding sources

The annual operating cost of NDIF is estimated to be about $0.5 million, which includes operations personnel and the cost of ongoing user training and support. This cost will be defrayed through future fundraising for research for which NDIF is a critical resource, and through a backstop funding commitment of $1 million from Northeastern Khoury College of Computer Sciences.

9.11 Evaluation

Project leadership will continuously evaluate the progress of the project towards the specific yearly goals enumerated in Section 3.2. In addition, each committee will continuously collect and monitor fine-grained metrics appropriate to its focus: **The outreach and training committee** gathers and analyzes user information including information on the diversity of users and workshop participants across demographic groups, career stages, geographies, and institutions, as well as research output including citations and major works. **The technical configuration committee** measures experiment throughput and latency, uptime, usage rates of capabilities and models, and error rates. **The open-source committee** monitors and analyzes bug reports, community discussions and pull requests, as well as issue response rates. The committee summarizes and reports on top community issues each quarter. **Other operating metrics** will be developed by the team as part of the service development process. All metrics will be tracked by project management continuously through dashboards and reviewed by the director and the advisory board on a semi-annual basis.

10 Broader Impacts

Understanding the impact of AI across society: LLMs are already being rapidly integrated into consumer products, and are impacting fields outside of CS (e.g., medicine [35]); their impact on society will continue to grow. LLMs have advanced so rapidly that some have called for a temporary pause on LLM development until academic research can catch up [142]. As discussed in Section 2, NDIF will provide the computing resources and training necessary for researchers to characterize benefits and risks of LLMs.

Democratic and equitable access to NDIF: Section 6 describes our outreach, training and support plan, which will ensure democratized access to NDIF. Our outreach plan is structured to build upon our established partnerships with Northeastern's Center for Inclusive Computing (led by co-PI Brodley), supplemented by collaborations with the Computing Research Association (see attached letter of collaboration from Tracy Camp). Our training and support plan will build a scalable network of experts across the country that can further promote the NDIF and help us understand the local needs of the different sites that we serve.

Workforce development: This project will directly contribute to the training of undergraduate, masters, and doctoral students who will be engaged in the development, operations, and evaluation of the NDIF. Building on our experiences designing project-based software engineering education, we will create course projects that engage students in NDIF development. We will make a special effort to engage students in Northeastern's "Align" masters program, which provides a direct pathway into computing for students without a CS background. Northeastern is well-known for experiential learning — every student completes at least one six-month full-time Co-Op — and will build on our existing efforts to recruiting students to develop software.

11 Institutional Commitment to Inclusion

Khoury College of Computer Sciences is a leader in broadening participation in CS. Khoury is home to the Center for Inclusive Computing (CIC) [143]), which aims to increase the representation of women of all races and ethnicities majoring in CS across the U.S. The CIC works with 100+ domestic institutions to remove institutional barriers to students discovering and excelling in computing. Under co-PI Brodley's leadership, Khoury piloted and scaled the Align Master's (MS) in Computer

Science program [144, 145], which provides a pathway to an MS in CS for students without CS backgrounds. This unique program attracts a notably diverse student body; in 2022 more than half of the incoming class were women and 20% of the domestic students identify as Hispanic, Latino, African-American, Native American, or Pacific Islander. In 2019, the CIC brought this innovation to other universities and established the MS Pathways Consortium [146], a network of 23 institutions now offering the MS in CS for non-majors. Khoury also has a verified college-wide broadening participation in computing plan [147].

12 Divestment

At the end of the lifetime of the facility, NDIF will archive its configuration, documentation, and source code in open-source repositories so that they remain available on GitHub.

13 International Collaborators

Our project does not involve international collaboration. International researchers can participate in our virtual communities, and can use NDIF through allocations with a U.S.-based PI.

14 Results of Prior NSF Support

PI Bau has no prior NSF support.

Co-PI Brodley is PI/Co-PI on four current NSF grants, all of which share the same **Broader Impact:** to increase the representation of populations historically minoritized in tech in the undergraduate and graduate computing populations. The award most relevant to this proposal is #2137907: BPC-DP: Distributed Research Apprenticeships for Master's (DREAM), (2021-2023, $300,000) supports MS students in the MS Pathways Consortium universities to participate in research. **Intellectual Merit:** The diverse demographics of the Consortium programs provide a unique opportunity to recruit Ph.D. students from a previously untapped population of students. This project has not yet resulted in publications.

Co-PI Wallace is PI on multiple active NSF awards; most relevant to this proposal is "RI: Medium: Learning Disentangled Representations for Text to Aid Interpretability and Transfer" (NSF 1901117, $999,990.00, 2019-2023). **Intellectual Merit:** The aim is to develop neural networks that yield *disentangled* representations, i.e., which factorize into interpretable sub-components. Such representations can afford *interpretability* by being explicit about what aspects of a text they encode. The project has yielded several publications describing progress toward these ends [39, 53, 117, 119, 123–125]. **Broader Impact:** The technical focus of this project—interpretabile neural networks via disentanglement—has clear implications with respect to fairness, as it provides mechanisms to inspect *what* models encode. The project has also supported undergraduate research.

Co-PI Bell's most relevant recent award is CCF-2100037 "SHF: Medium: Collaborative Research: Enhancing Continuous Integration Testing for the Open-Source Ecosystem" ($400K, 2018–2023). **Intellectual Merit:** This project addresses the problem of regression testing in the new setting of continuous integration (CI), and has focused on detecting flaky tests [135], understanding flaky tests [148–150], and making CI builds faster [151]. **Broader Impact:** This project has resulted in significant technology transfers to popular open-source projects Apache Maven [151] and Pitest [149], and creation of educational materials for CI [152, 153].

Co-PI Guha is PI on NSF Award "SHF: Small: A Language-based Approach to Faster and Safer Serverless Computing (SHF-2102288, $441,149, 2020-2022). **Intellectual Merit:** This project aims to develop new programming abstractions and tools for serverless computing. The project has produced several papers [130, 154–157]. Wasm/k [155] implements continuations for WebAssembly, a growing platform for serverless computing. **Broader Impact**: PI Guha is standardizing WebAssembly effect, informed by Wasm/k.

Name	Institution	State	MSI	Department	Expertise
Prof. A.A.	UC Berkeley / UCSF	CA		Computational precision health	ML for healthcare
Prof. J.A.	MIT	MA		Computer Science	NLP
Prof. S.B.	Brown University	RI (EPSCoR)		Computer Science	ML
Prof. K.B.	Boston University	MA		ECE	ML / Medical imaging
Prof. B.B.	Harvard University	MA		Computer Science	Theory
Prof. T.D.	Oregon State University	OR		Computer Science	ML
Prof. M.F.	Florida International University	FL	HSI	Computer Science	AI / Narratology
Prof. M.G.	MIT	MA		Computer Science	ML / Health
Prof. B.H.	University of Tennessee Knoxville	TN		Information Sciences	Disinformation
Prof. Y.K.	MIT	MA		Computer Science	NLP
Prof. J.L.	UT Austin	TX	AANAPISI/HSI	Linguistics	NLP
Prof. A.M.	University of Utah	UT		Computer Science	NLP
Prof. Z.M.	North Dakota State University	ND (EPSCoR)		Communication	Rhetoric
Prof. K.L.	University of Wisconsin Madison	WI		ECE	ML Systems
Prof. G.L.	NYU	NY		Psychology and Data Science	Neuroscience
Prof. S.P.	UC Berkeley	CA		Psychology	Cognition
Prof. J.R.	UC Santa Barbara	CA	AANAPISI/HSI	Computer Engineering	Computer architecture
Prof. Z.L.	Carnegie Mellon University	PA		Computer Science	ML / NLP
Prof. H.S.	University of Oregon	OR		Computer Science	ML / Vision
Prof. N.S.	University of Washington	WA		Computer Science	NLP
Prof. Y.V.	Columbia University	NY		Political Science	Politics and immigration
Prof. I.Y.	San Francisco State University	CA	AANAPISI/HSI	Computer Science	HCI
Prof. K.R.	North Carolina A&T State	NC	HBCU	Computer Science	ML / Security
Prof. V.B.	Arizona State University	AZ		Engineering & Health	Medicine
Prof. A.R.	UMass Lowell	MA	AANAPISI	Computer Science	NLP
Prof. E.P.	Brown University	RI (EPSCoR)		Computer Science	NLP
Prof. N.B.	Stony Brook	NY		Computer Science	ML / Systems
Prof. Y.L.	University of Nebraska Omaha	NE (EPSCoR)		Computer Science	NLP
Prof. A.R.	Cornell Tech	NY		Computer Science	NLP
Prof. B.D.	University of Florida	FL		CISE	AI / NLP
Prof. S.F.	Williams College	MA		Computer Science	Department Chair
Prof. N.F.	Cornell University	NY		Computer Science	Dean of Research
Prof. A.C.	Tulane University	LA (EPSCoR)		Computer Science Department	Social network analysis
Prof. R.M.	UT Austin	TX	AANAPISI/HSI	Computer Science	ML / NLP
Prof. L.G.	UC Santa Cruz	CA	AANAPISI/HSI	CSE	XAI
Prof. E.A.	UPR Mayaguez	PR (EPSCoR)	HSI	CSE	ML

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Alex Nichol, Alex Paino, Nikolas Tezak, Jie Tang, Igor Babuschkin, Suchir Balaji, Shantanu Jain, William Saunders, Christopher Hesse, Andrew N Carr, Jan Leike, Josh Achiam, Vedant Misra, Evan Morikawa, Alec Radford, Matthew Knight, Miles Brundage, Mira Murati, Katie Mayer, Peter Welinder, Bob McGrew, Dario Amodei, Sam McCandlish, Ilya Sutskever, and Wojciech Zaremba. "Evaluating large language models trained on code". In: *arXiv preprint arXiv:2107.03374* (2021).

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