Overview

Large language models (LLMs) such as ChatGPT that surpass 100 billion parameters have ushered in an exciting new era of artificial intelligence (AI). But their massive size has created a crisis of transparency; the computational requirements to run such models have made it infeasible for academic researchers to conduct research into how they work. To address this critical research need, we propose to design, build, and deploy computing infrastructure for **deep inference** in LLMs. 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.

The **National Deep Inference Facility (NDIF)** will advance scientific understanding by providing U.S. academic researchers with efficient, reproducible, and fully transparent access to the complete computations of pre-trained LLMs beyond 100 billion parameters—a capability not currently accessible to academics today. This facility will launch a new phase of AI innovation in the U.S., improve understanding of AI models, unlock cutting-edge advances and enable widespread training of a highly skilled workforce to lead the world in the ethical use of state-of-the-art LLMs.

Intellectual Merit

The National Artificial Intelligence Research Resource Task Force has identified the development of **trustworthy AI** as one of the critical priorities for strengthening U.S. Artificial Intelligence (AI) R&D. The NDIF directly addresses this national priority by providing the computational capacity, instrumentation, and transparency, as well as the broad access and training that is necessary to enable research on LLMs to advance trust, including investigations of societal implications, auditing of internal mechanisms, reproducible testing and evaluation, and studies of AI safety.

State-of-the-art machine language models trained to predict language use on large text data sets have exhibited new capabilities when models are scaled over 100 billion parameters, including some aspects of general-purpose reasoning [1]. The emergence of these capabilities has posed a wide range of **fundamental scientific questions that impact almost every discipline**. However, the ability to train LLMs does not directly lead to an understanding of how they are able to achieve such feats at inference time (i.e., when they are run). That hinders our ability to anticipate, explain, and regulate these systems. The NDIF addresses an urgent need for transparency.

With the collaboration of dozens of scientists nationwide and under the leadership of a unique team of experts in machine learning, deep network interpretability, language modeling, software engineering, high-performance computing, and inclusive computing, the proposed project will yield **open-source software, tools, and a broadly-available national computation resource for transparent LLM inference** to enable the U.S. academic community to conduct cutting-edge research into the mechanisms, limits, and impacts of state-of-the-art LLMs.

Broader Impacts

Highly-capable LLMs will increasingly be deployed into use, with potentially widespread implications for society [2]. *But scientists cannot explain the predictions of such models*. Although academics are well-suited to critically scrutinize the inner-workings of large AI models, the infrastructure required to perform such research is out of reach for most academic labs. The NDIF will enable U.S.-based academics to conduct critical research into LLMs that is currently not feasible, spurring broad advances exemplified by our collaborating researchers in **computing, medicine, neuroscience, linguistics, social sciences and humanities**.

The inference service and outreach will directly support the research agendas of graduate students in AI, thereby playing **a central role in training the next generation of researchers**. Moreover, we will develop undergraduate and graduate-level course materials and, through workshops and fellowships targeting PUIs and MSIs, make these resources broadly available across the nation.

Mid-scale RI-1 (M1:IP): The National Deep Inference Facility (NDIF) for Hundred-Billion-Parameter Language Models

This is a Mid-scale RI-1 implementation proposal. There are no anticipated environmental or cultural impacts.

1 A Computational Microscope for Large Language Models

Powerful large language models (LLMs) such as ChatGPT [3] herald a new era of artificial intelligence (AI) that is poised to reshape society [4], but *scientists cannot explain their predictions*. LLMs are able to write cogently about real-world topics [1], follow human instructions [5], and even pass legal [6], medical [7], and computer programming [8] exams. Both policymakers [9] and researchers [10] have stressed the urgency of explaining how they perform such tasks. Because we know how to *create* LLMs, we can now 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, AI researchers will explain machine intelligence by running LLMs under a computational microscope.

The need for national-scale instrumentation to explain LLMs arises due to the demanding computational requirements for conducting research-oriented inference on these very large models. *Training* LLMs requires massive computational resources using graphical processing units (GPUs) to analyze huge bodies of text. Once trained, LLMs are used for *inference*—i.e., the models are run with learned parameters. Inference still requires significant resources, as the trained model cannot fit onto a single GPU. While private companies like OpenAI offer black-box commercial inference services (Figure 1a) such as ChatGPT, those do not expose their internals, and it is impossible to study their mechanisms. By providing a transparent inference service (Figure 1b), NDIF will enable rigorous study of LLMs, increasing critical scientific understanding and supporting research on the impact of LLMs on society. The NDIF consists of three complementary investments:

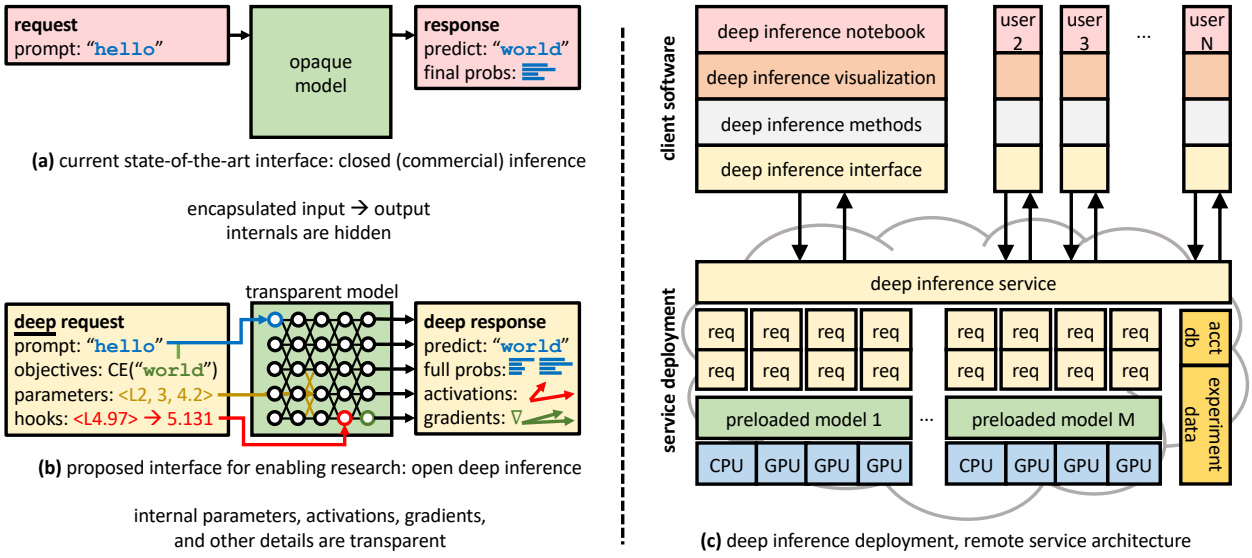


Figure 1: (a) Current services hosting large language models provide very limited interaction functionality (Top). One can send input text in a request, and is then provided an output string (and scores associated with the final predictions). (b) We propose developing infrastructure to provide deep access *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.*

1. Creation and testing of an online inference service with the support staff and infrastructure necessary to provide academics with the ability to interrogate and conduct groundbreaking research on the largest available and most scientifically relevant LLMs. (Figure 1c).
2. Development of an open-source server and client software stack that will power the service, suitable for deployment on other large clusters.
3. Outreach and training for PhD students and U.S. researchers to use this facility to advance understanding of large neural network models and their impacts.

NDIF is complementary to other projects—detailed in Section 2.2.1—that have the goal of *pre-training* open LLMs. Those efforts aim to produce LLMs with open parameters such as Bloom [11] and OPT [12], but they do not provide the inference service infrastructure that would be needed by academics to study them in detail. NDIF will provide academic researchers with that infrastructure. It will provide the computational capacity, software tools, and community support needed to run large, open, trained LLMs and perform transparent deep inference research on them. By "deep inference" we are denoting 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 will be developed at Northeastern University, building on our existing organizational structure, facilities, and experience in research computing. The hardware cluster will be deployed at the Massachusetts Green High Performance Computing Center, a shared computation facility, in which Northeastern is one of the five university partners.

Why not a traditional HPC cluster? There are a number of DoE and NSF funded clusters, such as those available from XSEDE/ACCESS, that allow U.S. academics to access accelerated computing hardware. However, whereas clusters are designed for batch jobs and partition resources across users, NDIF will be optimized for workloads where several users share access to a large model loaded into several GPUs. This will lead to much higher utilization and lower operating costs than a traditional cluster will allow.

2 Intellectual Merit

Explaining AI systems is a national and global priority: the National AI Research Resource Task Force [13] identified that one of the four critical opportunities for strengthening the U.S. AI R&D ecosystem is to develop 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." Similarly, the Future of Life Institute, whose "Pause Giant AI" open letter [10] has more than 25,000 signatories including many other leaders in AI, has recommended "a significant increase in public funding for technical AI safety research" in the areas of alignment, robustness and assurance, and explainability and interpretability [14]. And the White House Office of Science Technology Policy has released a Blueprint for an AI Bill of Rights [9] delineating a consumer's right to AI systems that "provide explanations that are technically valid, meaningful and useful."

Meanwhile, LLMs such as ChatGPT are being adopted more quickly than any previous technology, with widespread deployment in consumer-facing technologies [15], touching intellectual work in almost every field even as its mechanisms remain unexplained [4]. 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 to develop trustworthy AI.

Academic researchers are well-suited to investigate the mechanisms of LLMs, but for the reasons we shall detail in Section 2.2—primarily a lack of infrastructure—they are unable to do this critical research. The barriers to research are a new problem, largely stemming from the

unprecedented scale of state-of-the-art LLMs. NDIF will directly address these needs through a robust investment of a shared hardware and software platform. NDIF will enable a diverse community of researchers to conduct rigorous analysis of large language models to understand their inner-workings and failure modes.

2.1 Scientific justification

Since the emergence of computing as a discipline, researchers have pursued the creation of generalized or "human-like" machine intelligence, and debated how to measure it [16, 17]. Previous generations of AI systems have surpassed human-level capabilities in narrow domains such as playing chess [18], answering quiz-show questions [19], playing Go [20], and classifying images [21]. Capable as they are, those systems are qualitatively different from the emerging technology of LLMs, because LLMs are *generalists*. LLMs are able to perform a variety of tasks without additional explicit supervision [22], which makes them a uniquely interesting subject of study.

The flexible capabilities of LLMs that started to become apparent in GPT-2 [23] and GPT-3 [22] have emerged from pre-training with the simple and classical language-modeling objective of predicting the next word in a sequence, given the preceding words.[1] Despite this simplicity, LLMs such as GPT-4 [25] and OPT [12] are capable—to varying degrees—of answering questions about the world [26], translating between natural languages [22], performing mathematical reasoning [27], obeying descriptive requests to perform a variety of tasks [22], applying "theory-of-mind" reasoning about the knowledge of people [1], and learning to perform a new task given a small set of input examples without further training [22].

The purpose of the NDIF is to provide the broad academic research community with a platform to conduct experiments that explain the mechanisms and impacts of such emergent phenomena.

2.1.1 Large language models have created a new crisis of transparency

While the emergence of very large models such as GPT-3 [22] has energized the Natural Language Processing (NLP) and broader Machine Learning (ML) research communities, the dominant success of such models has also presented the research community with a crisis of transparency that is very different from the previous generation of "large-scale" AI.

When the AlexNet [28] model shocked the computer vision community in 2012 by winning the ImageNet Visual Recognition Challenge, it comprised 62 million learned parameters. That was large for the time, but sufficiently small for academic labs to be able to reproduce, validate, modify, retrain, and study the model using relatively cheap hardware. Similarly, when the first successful pre-trained models for NLP—e.g., ELMO [29] and BERT [30]—emerged, these were small enough for academic researchers to run, interrogate, and tinker with locally, enabling important research into their capabilities and limitations [31]. That accessibility led to an explosion of creativity and innovation, with a doubling of AI papers published annually from 2011 to 2021, and a 30-fold increase in the annual number of AI-related patents filed [32].

The current advance represented by GPT-3 [22] and similar very large language models (LLMs) is qualitatively different. The 175-billion parameter GPT-3 model is private. Alternative, comparably sized LLMs (such as OPT [12], Bloom [11], and NEO-X [33]) are technically available to researchers, but often *de facto* inaccessible due to their size: Most academic researchers do not have sufficient resources to run such models, and so they are unable to probe them in depth. Much

[1] GPT-3 and GPT-4 are understood to have also been "fine-tuned" using human feedback, but OpenAI provides practically no details on this [24], which is illustrative of their opaque modus operandi. The degree to which such explicit supervision is required to realize the impressive performance of LLMs is yet another open question which the NDIF will help researchers investigate.

academic work on analyzing LLMs therefore relies on the paid Application Programming Interfaces (APIs) that OpenAI or other vendors make available for integrating with other commercial products. Inference API services obviate the need for one to run (very large) models locally to interact with them. But this approach comes with a critical trade-off: Commercial inference APIs provide only limited access to model outputs (Figure 1a), in part to ensure that model weights remain proprietary. This precludes researchers from characterizing the internal mechanisms that models have learned from data, and that in turn threatens to slow the pace of innovation, shielding new developments behind the cloak of private ownership such that advances in AI cannot be subject to the kind of competitive scrutiny provided by independent academics.

Moreover, opaque models directly conflict with the aim of developing trustworthy AI. Our ignorance about the mechanisms that give rise to surprising LLM capabilities creates a troublesome dilemma between performance and transparency [34], making it difficult to anticipate how models will behave when deployed in the real world [35, 36]. Furthermore, our lack of understanding hinders our ability to regulate these systems and ensure safety [37, 38].

By enabling the diverse academic research community to scrutinize how such models work, the NDIF will empower important research into the potential risks of LLMs that are beyond the purview of industry labs. The broad range of academic researchers in our user community (Section 2.3) demonstrates that the NDIF will enable research not only in computer science, but also in biomedical science, neuroscience, bioinformatics, and social sciences. We should not leave critical research on LLMs—their capabilities, biases, functioning, and shortcomings—only to companies with clear self-interest in their reception. Such research should be conducted by academic groups in a transparent manner that emphasizes reproducibility and ethical conduct of research, and it should be subject to the rigors of peer-review.

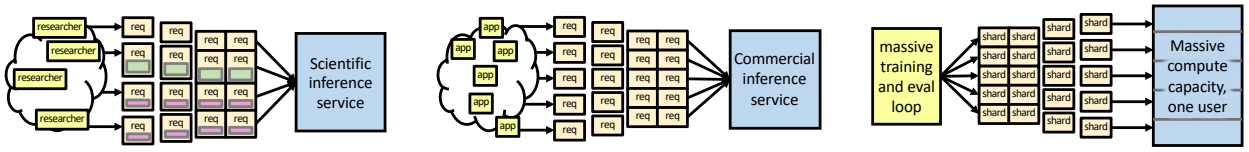
2.1.2 Research methods for understanding LLMs

The emergent capabilities of large models pose a fundamental question: *How do they work*? When a large model makes a surprising decision, what information contributed to this? What rules did the model apply to make its choice? What information has the model learned to store, and where does it put it? Understanding such mechanisms is important to distinguish profound computational capabilities from the mere *appearance* of them. The NDIF will enable several classes of experimental methods to enable researchers to characterize LLM mechanisms; we enumerate some in Figure 2. Here we provide more details on a few of these methods (we do not review them all in detail owing to space constraints).

Deep inference research methods on LLMs enabled by the NDIF	*Compute profile*			*Transparency needs*				
	Interactive	Batch	Optimization	Activations	Gradients	Interventions	Parameters	Training data
Human subject studies	✓			✓				
Representation probing	✓			✓				
Interactive visualization		✓		✓				
Saliency mapping		✓	✓	✓	✓			
Causal mediation analysis		✓		✓		✓		
Input synthesis methods			✓	✓	✓			
Parameter efficient fine-tuning			✓		✓	✓	✓	
Direct model editing			✓	✓		✓	✓	
Influence functions			✓		✓			✓
Representation similarity analysis		✓		✓				
Latent factor modeling		✓		✓				
Neuron response analysis		✓		✓		✓		✓
Memorization analysis		✓						✓

Figure 2: Deep inference research methods enabled by NDIF.

Representation probing. One major line of inquiry asks: What information does the network encode? For instance, computational linguistics might want to know whether and to what degree LLMs encode varieties of *semantics* [39]. This is illustrative of a body of emerging research probing internal representations for implicit linguistic structure (e.g., [40, 41]). Elsewhere, work on LLMs for healthcare has shown that neural representations of health records implicitly encode patient race; this has fairness implications [42].



Many users Inference with science payloads | Many apps Simple inference requests | One big user Terawatt-hour training job

(a) **NDIF**: scientific LLM inference facility | (b) Commercial LLM inference service | (c) HPC applied to LLM training

Figure 3: The computational workload of (a) NDIF consists of scientific inference requests which are small (e.g., sub-second) tasks with diverse scientific payloads that serve many different experiments. These differ from (b) commercial inference, which serves apps with no scientific payloads and also very different from (c) training LLMs on traditional HPC clusters, where a single user runs a massive job for months.

As another intriguing example, recent work found that even when a language model is conditioned to output falsehoods, it may contain a hidden state that represents the true answer internally [43]; this discovery is only possible with access to model internals.

Salience mapping. A model can also be better understood by asking: What parts of the input are most affecting its response? Saliency techniques aim to answer this question. These can be based on gradients, which can directly capture the magnitude of change expected in the output distribution as a result of small perturbations to inputs (or intermediate parameters) [44, 45]. Alternatively, one can analyze model *attention* distributions. In small models such analysis has revealed how simple dependencies are processed [46–48], including the discovery of very explicit copying circuits in transformer models [49]. Analyzing per-token model probabilities can reveal model self-knowledge [50] and differences between human and AI-generated text [51]. Extending these lines of inquiry to large models requires transparent access to model internals.

Causal mediation analysis. Another way emergent learned algorithms can be understood is through measuring the impact of modifying individual computational steps within a model. Such *causal* analysis has been applied to identify attention heads that mediate gender bias in language models [52]; indirect object identification in sentences that name multiple subjects [53]; and the recall of world knowledge within large language models, such as knowledge of the relationships, associations and properties of real-world entities [54, 55]. Using such methods to interrogate larger models requires direct access to internal states.

Parameter-efficient fine-tuning. One of the most compelling properties of large language models is their ability be quickly fine-tuned to a specific task using a small amount of data [56]. The NDIF will support investigation of such capabilities by supporting parameter-efficient fine-tuning methods such as *adapter layers* [57, 58], which are free parameters inserted into the network and then fine-tuned for a specific task while other network parameters remain fixed. This is a similar strategy to "soft prompts" [56], which similarly introduce a small set of tunable parameters, albeit in this case they are viewed as pseudo input token embeddings.

2.1.3 Computational profile of research methods for inference

The diversity of LLM interpretability methods make the computational requirements of such research unique, with a distinct access pattern that sets it apart from standard inference needs, and also from traditional high-performance computing workloads (Figure 3). Below we detail the unique computational profile that inference research requires and how this motivates novel infrastructure development.

Deep inference involves small, heterogenous requests with scientific payloads. The access pattern created by research on inference is characterized by running small inference requests

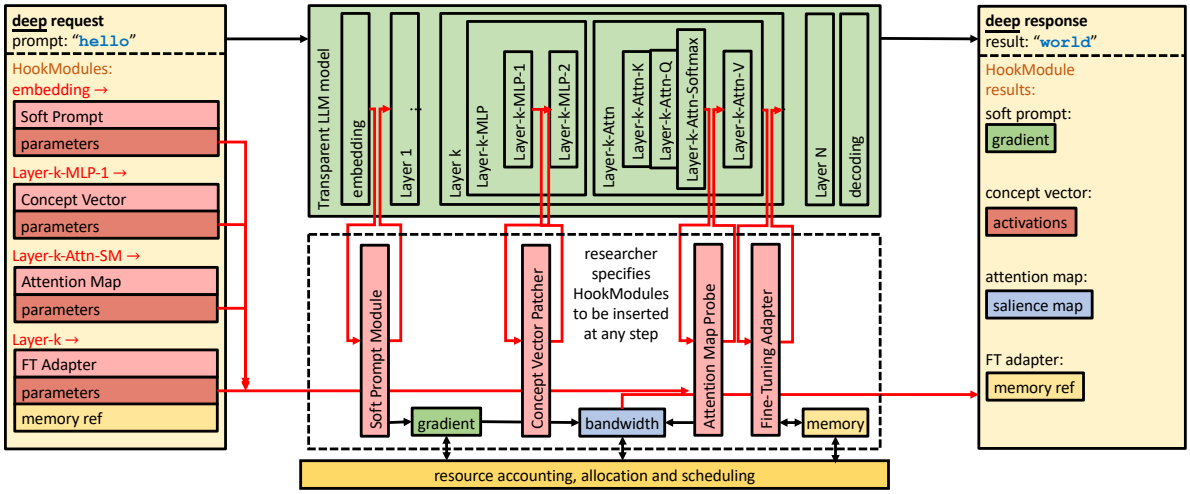


Figure 4: Details of the logical view of a deep inference request. Unlike commercial inference that provides no transparency, with the NDIF, researchers can execute flexible experiments by inserting computations in the internals of the deep network inference process. To maintain safe and efficient co-tenancy, experiment computations are packaged as `HookModules` *that enable resource accounting and scheduling.*

together with transparent access to various aspects of model computations, including activations, gradients, parameters, interventions, and original training data (see Figure 2). Because each experimental method can be decomposed into a small number of types of needed access, the research workload lends itself to a design in which users can submit streams of inference requests, each containing a modular specification of scientific payloads to attach to individual inference requests (Figure 4). While the scientific payload has a modular structure, the variety of different ways to apply and combine the modules creates a heterogeneous workload, where many requests may be inexpensive, but others may consume more memory, bandwidth, or computation.

This unique access pattern can also be divided into three major use cases: (1) Simple generative access that includes only lightweight scientific payloads for which it is possible maintain low latency; (2) Batch access, where the scientific payloads may be larger but real-time response is not needed; and (3) Optimization usage, where iterated calculations are done to calculate a statistic or optimize an objective. Support for these successively more complex categories of usage correspond to phases of the software development and deployment of NDIF, as we discuss in Section 4.1.1.

Commercial inference servers support only uniform requests. The workload of NDIF differs from existing non-research-oriented commercial inference services, although they resemble NDIF in some ways: they are structured with a service API architecture, serving a stream of small requests by running inference on a preloaded model. Like NDIF, these services amortize the cost of loading a model, and they achieve economies of scale by batching requests from many users together. However, unlike NDIF, they have no scientific payloads, so all the requests are similar and small. Commercially available inference APIs include: The OpenAI inference API providing access to OpenAI's GPT-3 and other large models; The Azure inference API, which offers several Microsoft-proprietary models; the Huggingface inference API; and the Cohere inference API, and the Amazon bedrock service. Because **the goal of our proposed service is to support fundamental research**, providing deep access to model internals, our inference service must provide additional functionality that is not available commercially, particularly the ability to manage scientific payloads safely and efficiently.

High-Performance Computing (HPC) facilities are suited to pre-training rather than inference. The compute required to support research into LLM *inference* is different from what *pre-training* such models demands. An inference research service must support multiple users making small, diverse requests to a shared pre-loaded model. In contrast, when pre-training a large model, a single job may run for many weeks or even months, executing the same training procedure in parallel across thousands of GPU devices. One job from a single user assumes complete ownership over a large model which it modifies on every iteration. Therefore, the compute infrastructure for pre-training need only support a small number of users accessing many nodes uniformly; this is a use-case well-served by existing HPC facilities.

The research workload of NDIF is different from traditional HPC workloads. It demands fine-grained flexibility, including the ability to accept and respond to a stream of very small requests from research users accessing the same models, and the ability to probe, inspect, and modify details of the pre-trained model to support the range of experimental methods as discussed above in Section 2.1.2. Because of these special requirements of deep inference research, the NDIF infrastructure will **not be used for pre-training models**. Unlike other machine learning infrastructure efforts, the NDIF is singularly focused on the infrastructure needed for *running* large-scale models to enable research on them *after* they are trained.

Enabling research into inference requires developing software that provides the desired functionality and access. In Section 4 we discuss development of open-source NDIF software, which could be deployed onto other clusters (i.e., in addition to our own). The NDIF will also provide open-source tools that will allow large-scale training clusters to support deep inference research if they choose to schedule inference service jobs rather than large-model training workloads.

2.2 Open Models: addressing the fourth barrier to understanding how LLMs work

Deep inference research on the largest language models such as GPT-4 [25] is hindered by four factors. The lack of (1) available **computational resources** for researchers, (2) open **inference software for research**, and (3) **transparency** with respect to the training data, architecture, computations, and parameters of the models. In previous sections we have spoken about the unique needs in these respects that the NDIF satisfies.

There is a fourth barrier to research on LLM inference that we discuss now: (4) the choice by companies to maintain **closed models** as proprietary secrets. While the NDIF addresses the first three of these needs, it does not address the fourth issue. That is for two reasons: firstly, as discussed in Section 2.1.3 the compuational demands of training are substantially different from those of inference, and we will focus on inference. Secondly, there are numerous other ongoing efforts to *pre-train* large open-models to address this fourth issue. We next survey other efforts to address the fourth need through pre-training open models, separate from NDIF.

2.2.1 Existing efforts to *train* open large language models with open parameters

The need for transparently trained 100-billion plus parameter models has been widely recognized by the research community, and several efforts are already in various states of progress toward this end. Concretely, currently available LLMs that we could make accessible at NDIF include:

- EleutherAI has released GPT-NeoX [33] and GPT-J [59], which are 20-billion and 6-billion parameter language models, respectively. (These were trained with support from Stability.AI, CoreWeave, and Google.) The Eleuther team plans to train a 150-200-billion parameter model. Eleuther has committed to make their parameters, code, and data available for use by academics on NDIF. We have attached a letter of collaboration from Stella Biderman, the Executive Director of EleutherAI; Biderman was also involved with the Bloom effort, described next.
- BigScience Bloom [11] is a 176-billion parameter multilingual model trained by BigScience, a

collaboration of European agencies, the Huggingface company, and many others.

- Meta OPT [12] and Llama [60], are families[2] of commercially licensed language models trained by Meta, with parameters that are made available to academic researchers. The OPT family includes a 175-billion parameter model and the largest Llama variant has 65 billion parameters.
- Tsinghua GLM is a 130-billion-parameter Chinese-English model supported by Zhipu.AI.

Further training efforts entail fine-tuning models to explicitly follow natural language instructions, similar to the functionality offered by OpenAI's InstructGPT and ChatGPT. For example, researchers at Stanford have released Alpaca [61], which is a version of the aforementioned Llama model fine-tuned with human instructions. Another example is BigScience BloomZ [62], which has fine-tuned Bloom with human feedback. Elsewhere, CarperAI [63] will fine-tune EluetherAI models. Large models with *multimodal* (e.g., vision and language) capabilities are also being trained; for example, the OpenFlamingo [64] project has begun releasing vision/language models derived from the Llama models.

In addition, several efforts are ongoing to create infrastructure to train even larger open models. These include government efforts such as the National AI Research Resource (NAIRR) [13], nonprofit organiazations such as the Large-scale Artificial Intelligence Open Network (LAION) [65], and private companies such as Together Computer [66]. This is a (very) fast-moving area, and we anticipate many additional publicly available large models to be available within the coming years; we (the PIs and the technical configuration committee, with input from external collaborators and community members) will regularly meet to make decisions about which models to add to NDIF, in order to maximize scientific impact.

Importantly, the above efforts to transparently train and make available LLMs are complementary to our goal. The proposed infrastructure focuses on addressing barriers to research at the *inference* stage; we do not aim to support large-scale training.[3] Despite the current and future availability of large models with more than 100 billion parameters, academic research that interrogates such models *after* they are trained will remain challenging because of the high cost of hardware and the complexity of software. NDIF addresses this problem.

2.3 Our research user community and illustrative application areas

The need for a large model inference service is widely recognized because the community has discovered that such models exhibit qualitatively different capabilities than small models. A recent survey of established benchmarks [67] catalogued over 175 different capabilities that emerge in large models but that do not appear in smaller models. These include the ability to perform multi-digit arithmetic, unscramble words, and correctly select truthful answers when baited by commonly-stated misconceptions. An illustrative and particularly intriguing emergent behavior that has been recently discovered is that LLMs can perform multi-step reasoning when prompted to do so [68, 69]; smaller LLMs do not seem to have this capability. Another striking characteristic of very large models is that they have been observed to perform well under domain shift [70].

Support for the specific NDIF proposal is strong in the community. In December 2022, we created a Twitter thread asking researchers to respond if they had work that would be enabled by a transparent national inference service for LLMs. Over 400 researchers indicated that the proposed NDIF service would support their research. Many emphasized the strong need for such infrastructure given the practical difficulties of investigating models whose parameters do not fit

[2] By this we mean there are versions of these models of varying size in terms of model parameters.

[3] We will support work on *parameter efficient* fine-tuning methods, because the question of how best to adapt LLMs to new tasks with minimal effort and training overhead is an active topic of research. However, such efficient fine-tuning is very different from large-scale *pre-training*.

into the memory of a typical research computing node. 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) saids, "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 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."

To better understand the needs of this target user community, we have established an active research community that includes 40 professors from 34 different universities in 19 states (including 6 EPSCoR states, Figure 5 and 8 minority-serving institutions (including an HBCU) who have suggested specific research projects that will benefit from NDIF. These projects span a broad range of topic areas. Here we provide illustrative, concrete examples of how a diverse set of academic researchers will directly benefit from the NDIF infrastructure.

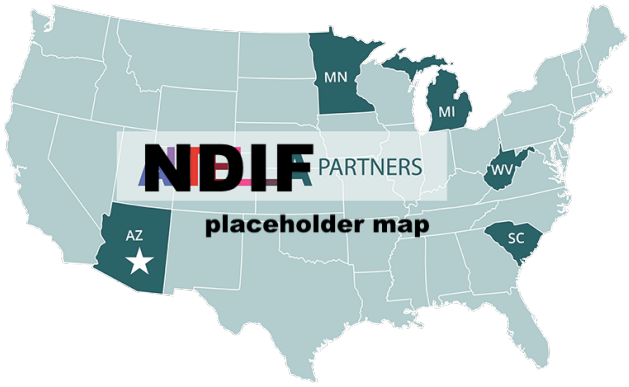


Figure 5: National reach: professors in the NDIF community who have proposed specific research projects to conduct with NDIF represent 34 universities in 19 states, including 6 EPSCor states.

Computational linguists and natural language processing (NLP) researchers are keen to understand the linguistic knowledge implicitly encoded in LLMs [71–73]. This subcommunity is also interested in the degree to which such models encode bias [74, 75], especially in sensitive domains such as healthcare [42, 76]. There is also a quickly growing sub-community investigating the mechanistic inner-workings of LLMs, perhaps best represented by the BlackboxNLP workshop [77], which has been held annually at ACL conferences for the past four years.

Computational linguistics and NLP researchers form a core constituency of enthusiastic would-be NDIF users, and representatives of this group have been actively taking part in design discussions accordingly. However, we stress that the NDIF will benefit researchers from a diverse set of academic communities, especially as LLMs begin to impact these fields—a few examples follow.

Social and political scientists we have spoken with are interested in the use of LLMs as tools for judging public opinion in ways that would be impractical to scale using other means [78], as well as using them to measure political ideology and other latent constructs from texts [79], and applying LLMs to various "text-as-data" tasks to permit subsequent analysis [80].[4]

Neuroscientists would like to use the NDIF to analyze artificial neural networks using tools from neuroscience [81, 82]. This research will have implications for both AI and the brain. LLMs have

[4]Some of these research settings may require only simple inference, at least for now. However, subtle but critical details preclude relying on proprietary and closed APIs such as that provided by OpenAI for science in these areas. For example, to ensure reproducibility for anything involving stochasticity (such as sampling), it is important to be able to set random seeds. Longer term, we anticipate that insofar as such models are adopted into the practice of, say, political science research, it will become increasingly critical to understand the implicit biases of such models—exactly the kind of Deep Inference research the NDIF will support.

the advantage of being decidedly easier to open, inspect, probe, and manipulate than brains, but only if infrastructure like the NDIF exists to permit such experimentation.

Researchers in healthcare are interested in a range of applications of LLMs [83]. For example, community members we have spoken to are investigating the use of LLMs to detect dementia from patient-elicited speech [84]. Other researchers we have spoken to are interested in studying how (health-related) domain knowledge is stored in LLMs, which will require deep inference. And then there are the critical issues related to learned representations and fairness [42] as well as risks of training LLMs on potentially sensitive personal health data [85]. Investigating such issues requires access to model activations and parameters.

The above is only a small and illustrative subset of the potential use cases across fields that we have discussed with researchers in this formative period. As LLM technology continues to impact new fields, so too will the need for rigorous LLM science which is not, in general, possible to conduct using commercial inference APIs.

3 Preliminary Activities

We have accomplished several preliminary tasks including recruiting prospective leadership staff, forming an open design process, outreach to relevant research community members, identification of goals, and preliminary development of technical plans.

3.1 Identification of goals together with the user community

As a facility intended to serve the needs of the wider community of researchers interested in LLMs, it is essential for the development team to have an intimate understanding of the likely needs of users of the facility, who will be pursuing a diverse range of research programs. Towards this end, have established on online Discord server devoted to design discussions, involving over 50 active researchers from universities across the nation pursuing LLM research across various fields including computer science, neuroscience, political science, and biomedical sciences. This forum is open to all prospective users of the NDIF and will serve as a direct conduit between our development team and the wider LLM research user community. We use the forum to conduct regular design discussions, enabling us to set priorities, gather detailed requirements, and validate development plans. Working directly with our user community, we have identified three core goals that will drive the detailed design of NDIF:

1. The facility will enable research into the most capable state-of-the-art open large language models as well as large multimodal models after they are trained.
2. It will provide full transparency and reproducibility, including access to model internals such as activations, weights, overrides, gradients, and the ability to control random seeds.
3. The NDIF will prioritize community support, with a focus on enabling academic researchers studying the mechanisms and impact of large language models in practice.

Our user community has made significant progress towards identifying capabilities that should be enabled by the facility after full deployment. Specifically, we have identified a list of experimental methods applied to neural systems that are a priority for our community (Figure 2). Furthermore, the community has begun to characterize key unknowns and available resources and has started the process of prioritizing detailed research capabilities to enable in the first phase of development.

In addition to reaching out to and connecting wtih potential NDIF users online, we have hosted an in-person outreach event at the International Conference on Learning Representations (ICLR) 2023. Our event brought together over 100 members of the machine learning research community to discuss challenges faced by researchers studying LLMs on academic budgets. During the event we identified a range of research priorities that will need to be addressed by the NDIF, and we

recruited researchers to participate directly in our user community.

3.2 Leadership recruitment

We acknowledge the challenge of attracting highly-qualified professionals in this field, and we are fortunate to have recruited two exceptional individuals who could be available to join our leadership team pending the funding of the project. William Brockman, PhD in Mathematics from UC San Diego, has led software development projects at top organizations such as Google, the Broad Institute, and General Dynamics. Brockman has been participating in our design process and helping to develop our technical specifications. If the NDIF is funded, could be available to serve as our lead software engineer. Sumeet Multani, PMP, holds a Master's Degree in Computer Systems Networking and Telecommunications from Northeastern University, and has served as a technical program manager at Google, TripAdvisor, and Akamai Technology. If the project is funded, Multani could be available to serve as our project manager. Both Brockman and Multani are based in Boston. Their roles in NDIF are described in Section 4.2.1.

3.3 Prototype and specification development

Working with the community, we have developed several small-scale prototypes that implement aspects of the NDIF service model. These include a software package used for instrumenting single-GPU neural networks that we have validated and used for several published research works, as well as a prototype web service to run research-oriented inference on a multi-GPU language model at a scale suitable for use by a single lab. We have used what we have learned from these prototypes to inform an architectural specification for NDIF. An overview of this preliminary specification is given in Section 4.1, and the specification is included in supplementary materials.

4 Implementation

4.1 Technical Readiness

Our team has developed a detailed technical specification and development plan that delineates the key requirements for the NDIF user model, software requirements, hardware design, deployment milestones, and team structure. We give an overview of this specification here.

4.1.1 Major Deployment Milestones

Our development and deployment of NDIF will proceed in several phases. The plan increases the maturity of all aspects of the facility in parallel, in order to deliver value to researchers as early as possible and maximize opportunities for project leadership to respond to user feedback and outside events during project development.

Pre-funding pilot, Summer 2023. Develop single-server cluster that can serve user requests and streaming interactions on medium-sized models. Preliminary client library with 5 local users.

Closed pilot, Q1 2024 (Year 1). First phase hardware (see next section) serving sustained research queries observating and modifying the largest models of interest, with both streaming and batch-oriented use patterns. Documentation is complete enough for early users. User audience: 20 selected early adopters drawn from our design-participant user community, working directly with our team and supported by our engineers and researchers.

Open pilot, Q1 2025 (Year 2). Second phase hardware enables opening up early access to qualified users at any educational institution, with limited support and no guarantees. Increased robustness, including monitoring and alerting, improved job queuing, and a fairness-oriented scheduler that protects the compute facility from abuse and accidental overruns. We define Service Level Objectives (SLO)s and measure progress towards meeting them. Optimization and gradient use

cases are available in preliminary form. Documentation is complete enough for early adopters, and draft tutorials are prepared.

Software API full release, Q1 2026 (Year 3). Robust support for optimization and gradient methods. Initial support for user-defined optimization and aggregation on-cluster. All major user-facing features of the system meeting robust SLOs. Documentation is complete and undergoes user testing and improvement. We will teach 100+ research users how to use the system in a large multi-site bootcamp.

Operations scale-up, Q2 2027 (Year 4). Refresh hardware to support new models, larger models, more models, and more users. Continued refinement of ability to onboard new users. Robust user-defined on-cluster computation. Refine system administration tools to improve issue response and stability. Pilot ability to run NDIF on other clusters and to route traffic to other HPC clusters.

Cluster self-hosting, Q2 2028 (Year 5). Administrative tooling is complete and robust enough to support distributing NDIF software to other HPC clusters. Hire permanent director, release major code version, prepare for sustained operations.

4.1.2 Hardware Design and Scale-Out

A key to the success of NDIF will be providing a high level of computational performance to enable rapid progress on impactful research. Optimizing the computing hardware to the unique needs of this workload will be critical. The core capabilities enabling scaling up model size are GPU VRAM and connection bandwidth between the GPUs. Therefore we plan our hardware build-out in three phases, to benefit from the rapid progress of GPU hardware driven by general AI workloads, and to be prepared to adapt to future developments in state-of-the-art models.

175-Billion Parameter Capacity, Q4 2023 (Year 1). The first phase of the hardware build-out is sized to match the current state-of-the-art: there are two open-parameter models at the 175-billion parameter size (similar to GPT-3), and we anticipate one more to be released soon. Thus we plan 10 nodes, each containing 640Gb of VRAM via 8x Nvidia 80GB A100 GPUs. This suffices to run three different models of this size, with three inference servers each, and one spare to reduce downtime.

500-Billion Parameter Capacity, Q4 2024 (Year 2). The second phase of the hardware build-out is to expand with 6 nodes, each containing 1.2 terabyes of VRAM, for example, through 16x Nvidia 80GB A100 GPUs. This will provide enough capacity to serve one 500-billion parameter model (five inference servers, with one spare node to reduce downtime). Currently the only models at this scale are proprietary, but we anticipate the availability of open models in this timeframe.

Trillion-Parameter Capacity, Q4 2026 (Year 4). The third phase of the hardware build-out is to expand with 4 nodes, each containing 2.5 terabyes of VRAM, for example, through 32x Nvidia 80GB A100 GPUs. This will provide enough capacity to serve one 1000-billion parameter model (three inference servers plus one spare node). This size matches the design goals of the NAIRR [13] public AI training resource.

The hardware rollout must be phased because commercial vendors do not currently offer 1.2 terabyte or 2.5 terabyte VRAM nodes. Nevertheless, those configurations are clearly on the horizon, for example Nvidia has tested 1.2 terabyte nodes. Our budget estimates the cost of those nodes by including quotes for sets of nodes that would contain the same major components.

4.1.3 Software Stack and Service Architecture.

The software layer is equally important to the success of NDIF. Its responsibilities face two ways: looking inward, it needs to promote efficient utilization of the hardware investment. Looking outward, it needs to provide smooth on-ramps and highly productive steady-state usage patterns

that enable experienced and new researchers to start working on the NDIF, come up to speed rapidly, and do effective and efficient scientific work addressing diverse research goals.

Inference backend. The workhorse of NDIF is the single-node multi-gpu inference backend. It enables efficient utilization by aggregating the stream of incoming inference requests into batches and executing the models, including all scientific payloads. It loads models, assembles batches of requests as tensors, instruments the model according to scientific payloads, tracks the association between individual experiments and batched data, manages movement of data between gpus including pipelining, manages the calculation of gradients, and tracks resources used. The inference server will be built using the open-source Nvidia Triton [86] inference server framework, with a custom-built backend for handling LLM scientific payloads with diverse access patterns and heterogeneous resource use.

Request router and scheduler. As inference requests arrive, the router is responsible for queueing, ordering, and routing those requests based on availability and prioritization. In the initial pilot, a naive (FIFO) scheduling algorithm is implemented, but in subsequent milestones, an adaptive scheduler will be developed to sort and group different classes of usage to improve utilization, and to maintain fair resource allocation across the cluster.

Optimization cache manager. To reduce the bandwidth consumed by stateless operation of common operations, NDIF will support data caching on each node. The optimization cache manager will manage all temporary storage and caching of user data, including, managing queues and cached intermediate results. The cache manager tracks cached data that may be present on any node, and it is able to orchestrate movement of data between nodes when needed. The optimization cache is essential for speeding up operations like gradient descent.

Administrative tooling. Administrators and engineers will develop a set of tools for maintaining a robust facility, inlucing logging and monitoring software, and tools and scripts for administrative tasks, including user administration and moderation, quota management, cluster model allocation, health monitoring, load monitoring, and debugging tools for inspecting activity on the cluster.

User interface frontend. This webserver forms the boundary to the user-facing aspects of NDIF. It includes the end-user visible views of the system, including signup, login, experiment console pages, as well as an interactive interface for directly conducting experiments with a model. It will support an HTTPS JSON API for submitting inference experiment requests and receiving results, to enable the community to integrate other systems using any language or framework.

Client-side Python API. The primary way researchers will conduct experiments will be through an open-source python library built on the `PyTorch` [87] deep learning framework that runs on the user's workstation. This library will provide a modular way to conduct LLM experiments, as shown in Figure 4, while supporting remote inference on NDIF models. The design priority is to provide a practical and accessible "on-ramp" for researchers to do research on LLMs.

Experiment methods library. Built on top of the core python API, we will provide modules that implement higher-level algorithms, interactions, analyses, and visualizations to implement the important experimental methods for various lines of LLM research.

All our software will be open-source and developed in public repositories, and will be developed with the active engagement of the user community and open-source contributors.

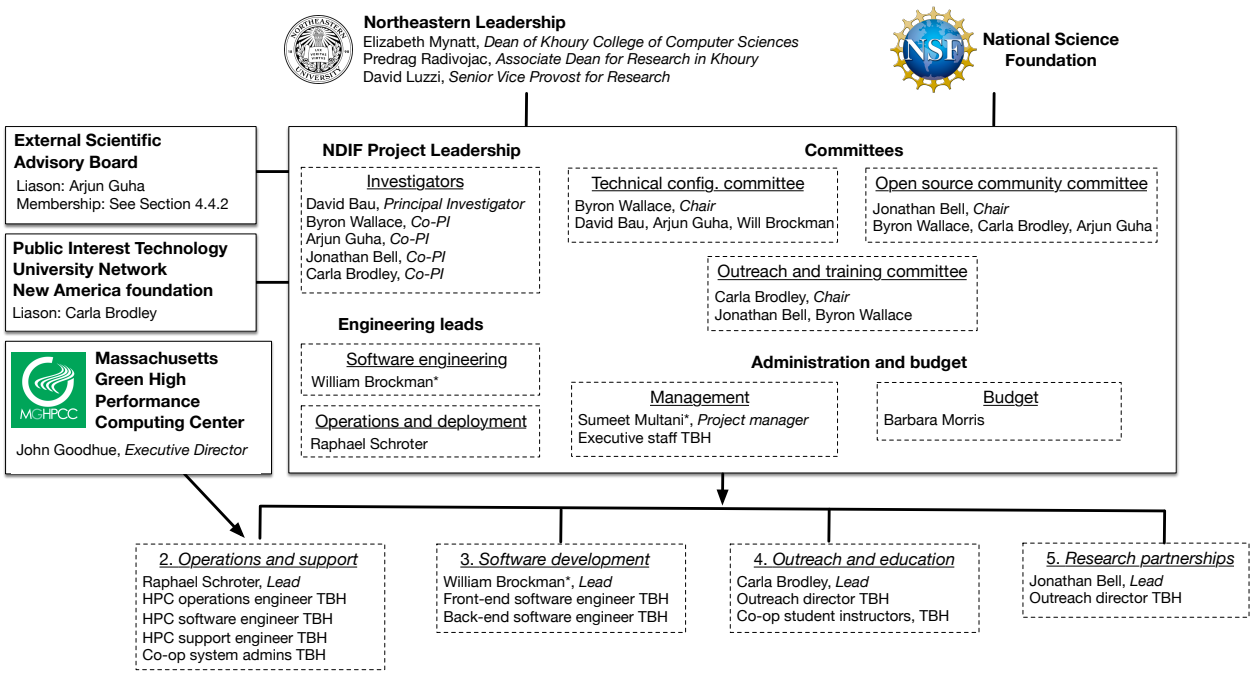


Figure 6: NDIF organization. Asterisks (*) indicate tentative hires.

4.2 Planned Project Management

4.2.1 Key Personnel

The organizational chart is in Figure 6. This project brings together an interdisciplinary group with deep expertise in machine learning (ML)/natural language processing (NLP), programming languages, software engineering, and large-scale computing, as well as experience in the development and operation of large-scale computing systems and the creation and administration of multi-institution research programs.

PI Bau (Assistant Professor in Khoury College of Computer Sciences at Northeastern) is a leading researcher in interpretability of large neural networks [88–91] and editing of large models [92–94], and he has been a pioneer in the explicit characterization of causal computational mechanisms within language models [54, 55, 95]. Bau also has a proven track record of creating and deploying large-scale projects at top technology companies; he created and managed the teams that developed realtime Google Image Search, Google Hangouts, the Pencil Code educational system, Weblogic Workshop for BEA Systems, and Apache Foundation's XML Beans. Bau also served as technical leadership on Microsoft Internet Explorer and Microsoft ASP.NET.

On the NDIF project, Bau will serve as Principal Investigator. In this role, he will hire and manage project leadership, as well as oversee the direction, development, and overall success of the facility. Bau will work closely with the project manager and lead software engineer to oversee the development of the project, and he will run monthly meetings of the NDIF leadership team. He will also serve on the technical configuration committee.

Outreach Lead and Co-PI Brodley (Dean of Inclusive Computing at Khoury and Founding Executive Director of the Center for Inclusive Computing at Northeastern University) 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 machine learning research has advanced computer science as well as remote

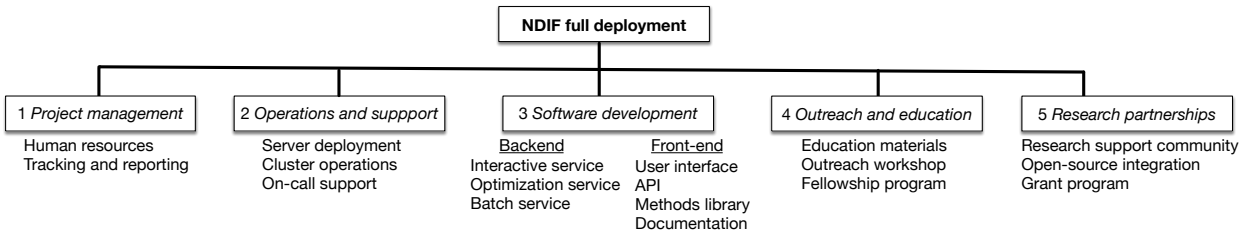


Figure 7: The work breakdown structure of NDIF construction.

sensing, neuroscience, digital libraries, astrophysics, image retrieval, computational biology, chemistry, and evidence-based medicine. Brodley will lead outreach efforts (WBS 1.4) and ensure broad participation in setting research priorities and the educational mission of NDIF. She will chair the outreach and training committee, which will meet quarterly and more frequenty as-needed to review and plan outreach work. She will serve as liason to the public interest technology university network, and she will serve on the open-source community committee.

Technical Configuration Committee Chair and Co-PI Wallace (Sy and Laurie Sternberg Interdisciplinary Associate Professor in Khoury) has extensive research expertise in NLP and interpretability of such models [96–103], as well as the use of NLP in biomedical settings [85, 104–107]. Wallace will chair the technical configuration committee, which will meet quarterly (and more frequently as needed) 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 Natural Language Processing and Biomedical research communities. He will serve on the open-source community committee and the outreach and training committee.

External Advisory Board Liason and Co-PI Guha (Associate Professor in Khoury) brings deep experience in programming languages, including language-based security [108–111], GPU accelerated domain specific languages [112, 113], and pre-trained models for code generation [114].

Guha will serve as liason for the External Scientific Advisory board. He will be responsible for engaging and recruiting leaders of the academic community to the external board; he will run twice-annual meetings of that group to ensure that the long-term needs of the academic community are met by NDIF. Guha will also serve on the technical configuration committee and the open-source community committee.

Open-Source Chair and Co-PI Bell (Assistant Professor in Khoury) is an expert in software engineering and systems, including architectural design [115], testing and continuous integration [116–119], and analysis [120–122].

Bell will chair the open-source community committee, which will meet quarterly and more frequently as-needed. He will be responsible for incubating the open-source community and overseeing open-source activities, and providing academic oversight on open source policies, technical contributions, and quality assurance. He will serve on the outreach and training committee.

HPC Operations Lead Schröter (Director of Research Computing at Northeastern University) organizes strategic planning for research computing resources at Northeastern; he works with university researchers across all disciplines, to achieve research goals using HPC infrastructure.

Schröter will manage deployment and operations for NDIF (WBS 1.2) and supervise the staff of HPC engineers. He will be responsible for managing the physical colocation of the facility, as well as day-to-day operations of the computing service.

Project Manager Multani (tentative) has extensive experience leading the definition, planning, and execution of both user-facing and infrastructure projects and has served as a technical program manager Google, TripAdvisor, and Akamai Technology.

As project manager, Multani will work closely with the PI, as well as all fourork areas of the project (WBS 1.1-1.5). He will be responsible for schedule management, budget management, scope management, and risk management. Additionally he will be responsible for all NSF reporting, including monthly reports, quarterly reports, annual reports, and periodic PEP updates.

Lead Software Engineer Brockman (tentative) has a wealth of experience leading projects in high performance computing, data science, and mathematical modeling, and has led software development projects at Google, the Broad Institute, and General Dynamics.

As lead engineer, he will be responsible for hiring staff engineers, and for managing the development process (WBS 1.3). Brockman will serve on the technical configuration committee.

4.2.2 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 no fewer than five and no more than ten members, and each member will be a subject area expert or a representative of a relevant constituency such as a university administrator. The following have offered to serve as initial board members:

Thomas Dietterich Distinguished Professor (Emeritus) and Director of Intelligent Systems, at the School of Electrical Engineering and Computer Science at Oregon State University. Dietterich is one of the pioneers of the field of Machine Learning and has authored more than 225 refereed publications and two books.

Alexander Rush is an Associate Professor at Cornell Tech, where he studies natural language processing and machine learning. He is also a researcher at HuggingFace, a leader in open-source natural language processing systems.

Steven Piantadosi is an Assistant Professor in the Department of Psychology at University of California Berkeley, where he is head of the COLALA computation and language lab. His research studies how people learn language and create conceptual systems.

4.2.3 Engaging the Public-Interest Technology Research Community

The benefits of advances in AI have been realized unequally [123]. To ensure critical assessment of the potential impact of LLMs on education, policy, privacy, and safety we will regularly engage with academics who work in the public-interest technology sector. We will work with New America's Public Interest Technology University Network (PITUN)[5] to bring both AI and non-AI faculty to workshops with AI researchers/students to discuss issues of interest. PITUN has a membership of 63 universities and colleges, 19 of which are Minority Serving Institutions (MSIs). PITUN will support the National Deep Inference Facility by establishing a PIT Advisory Group to provide guidance on the responsible and ethical design, development, deployment, and use of LLMs with an interdisciplinary approach that includes experts from both technical and social sciences.

PITUN will establish a PIT Advisory Group comprised of 10-15 interdisciplinary experts from PITUN to provide guidance on the responsible and ethical design, development, deployment, and use of LLMs. PITUN seeks to align PIT with both informal and formal STEM learning through

[5]See the letter of collaboration with PITUN. New America, founded in 1999, is dedicated to renewing the promise of America by continuing the quest to realize the nation's highest ideals, honestly confront the challenges caused by rapid technological and social change, and seize the opportunities those changes create. Its public interest technology program concerns the application of technology expertise to generate public benefits and promote the public good.

the capacity development of its 63 member universities. By undertaking the LLM project, PITUN aims to meet the following goals:

- Engage conversations regarding LLMs to be community-driven;
- Promote equitable and broad participation in the emerging field of AI through LLMs;
- Advance the knowledge base of LLM learning by advancing PIT with formal reports out from New America based on substantial feedback from semi-annual (or quarterly as needed) roundtables of its Advisory Group;
- 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;
- Develop professional capacity within member universities themselves to deliver informal AI learning using the LLMs within a PIT framework;
- Host an annual webinar to distill key findings and build a base of new AI learners through exposure to PIT and its applications in relation to LLMs.

4.2.4 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 choices will be made in consultation with the external Scientific Advisory board and the open source community.

After each phase is released for usage in phase 2 and beyond, agile project management methods will be adopted to continuously test the product to identify and solve problems, to iteratively improve the software and infrastructure. We will monitor customer-reported issues, cluster efficiency, and open-source contributions.

The technical configuration committee will conduct an annual review to identify changes in scope and determine where corrections are needed.

4.2.5 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 the NSF with the most current cost estimate for both capital costs and soft costs. We set $900,000 (5% of the total direct cost) as the budget contingency. This contingency 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.

4.2.6 Schedule and Schedule Contigency

The project will run from 9/1/2024 to 9/1/2029; please find the schedule in the PEP. In each year of the project we schedule a single major deployment release to increase the experimental capabilties of NDIF. After each of these releases, we set aside two months schedule contingency. If the schedule is followed, we will use these two months to collect customer feedback and focus on design review for the next phase. If not, the contingency allows time for unanticipated integration, performance tuning, quality assurance, or adjustments in scope. In that case, the project manager will conduct a program review to adjust scope, timing and budget of the project.

4.2.7 Risk Management

Our project will use the following process for managing risks

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. Possible mitigation include risk avoidance, risk transfer, risk reduction, and risk acceptance. Risk will be tracked over time, and the effectiveness of the risk-management process will be tracked.

In annual reviews, the project leadership including the PIs, project management, operations lead, and lead software engineer will conduct a comprehensive review of risks. As the project proceeds, each risk will remain on the risk register until it is closed. In addition, each risk will be reviewed by the team to understand methods for mitigating the risk. We have conducted an initial risk assessment; please 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 has been designed to mitigate those risks where possible.

4.2.8 Configuration Management

Changes for all project specifications other than software, such as specification of required infrastructure capabilities, hardware specifications, 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. They will utilize software version control through git, and all changes will go through code review. Unit testing will be conducted before changes are committed, and integration testing will be conducted before any changes are deployed to customer-facing services. All deployments will be given a release number, and a change log file will be maintained.

5 Operations and Utilization

After the successful deployment of NDIF, the organization will transition to ongoing operations. The primary focus will be to maintain the high performance computing infrastructure and ensure its continued availability to the research community. To achieve this, several key personnel and operational changes will be implemented.

5.1 Operations Management and Governance

In the final phase of development, the organization will hire a full-time facility director, who will be responsible for overseeing science operations. The facility director will ensure that NDIF continues to provide cutting-edge computational resources to researchers, as well as coordinate with other facilities to share best practices and advance the field. NDIF will also continute to maintain an external advisory board consisting of members of the scientific community and policy community from outside organizations. The advisory board will advise on allocation priorities, ethical issues, and strategic direction of the facility. The operating staff will include an outreach director who will continue to update educational materials and run workshops, and engage with the research community to ensure that NDIF remains accessible and user-friendly. It will also include a staff of software engineers who will be responsible for maintaining the software, responding to open-source contributions, and incorporating updates to keep up with the latest science.

Finally, NDIF will continue to fully staff system administration and operations. As a mature application, NDIF application-level system administration staff will transition to report into Northeastern Research Computing alongside HPC operations at MGHPCC. The HPC staff will maintain a high level of service for NDIF, updating software and making hardware repairs, and responding to operational issues.

5.2 Operating Costs and Funding Sources

The annual operating cost of NDIF is estimated to be about $2 million, which includes personnel, the cost of conducting outreach, and the cost of maintaining the hardware at the deployed level of computation. This estimate does not include any investments in increases in capacity.

The organization will ask the NSF to cover the annual operating costs of NDIF. Additionally, the organization will aim to defray some costs through a research partnership program, where researchers can contribute funds to the facility in exchange for access to priority scheduling queues. This program will help to ensure the long-term sustainability of NDIF and its continued availability to the research community.

5.2.1 Access and Utilization Plan

The NDIF will be open to all people with an educational affiliation to use, free-of-charge (using the NSF and DOE-supported "CILogon" Service for authentication). To allocate scarce resources when oversubscribed, we will implement an online adaptive scheduling algorithm that estimates and monitors heterogeneous resource use in order to fairly distribute computation, bandwidth, and memory. Based on our estimates of computing capacity of a state-of-the-art software implementation using our hardware configuration, we estimate a user will be able to get 10 tokens-per-second latency under light load (with 30 simultaneous users per node, when scientific payloads do not require smaller batch sizes). When usage is heavier or when users are placing sustained scientific load on the service, latency will naturally rise as capacity saturates, and heavy users will have their requests queued so that overall capacity is distributed equitably.

Paid Partnerships: the NDIF will also offer a paid "NDIF Partnership" program to allow researchers to subsidize capacity that they can allocate for sustained high-bandwidth usage for their research. For example, partnership fees can be paid for by researchers' grants, and they will give partners access to their own allocated queue where they can be assured of a level of throughput that is independent of baseline load on the public scheduling queue.

Need-Based Resource Grants: to ensure the broadest possible access to researchers who may have high computing needs without a source of sufficient funds enroll as a paid partner, NDIF will also award "NDIF computing grants" that will provide free-of-cost access to allocated high-bandwidth queues. We will broadly advertise these computing grants, particularly to new PIs, to PIs in EPSCOR states and to PIs at minority serving institutions. A competition for NDIF computing grants will be on a regular basis, and a committee appointed by the NDIF leadership will review and choose grantees based on need and scientific merit.

5.3 Evaluation

During both deployment and ongoing operations, We will continuously evaluate the project, both at the component-level (e.g. latency of individual APIs), and at the full facility-level. Our project is driven by four measurable goals:

1. **Advance scientific understanding** of large language models.
2. Provide **broad access** to researchers and students for inference not served elsewhere.
3. Enable **efficient use** of scarce computational resources.
4. **Train students** on large models, to build the next generation of AI engineers and researchers.

These goals correspond to metrics that we will track. To measure our progress in realizing **impact** by providing **broad access** and **efficiency**, we will track and aim to increase:

- **Sustained server utilization** in the deployed service, a core measure of efficiency. Our aim is to size the facility to maintain an overall utilization of 50% or more.
- **Experiment response latency** which quantifies the technical accessibility of the facility to researchers. The goal will be for latency to be low enough to enable interactive human studies with real-time interaactions with large models.
- **Number of monthly academic users** of the deployed service, a core measure of reach, along with metrics of the diversity of those users.
- **Number of peer-reviewed research works** that use our service or software in experiments.
- **The number of deployments** of our software stack on clusters beyond the initial service.

In addition, other operating metrics will be developed by the team as part of the service development process. These metrics will be tracked by the project continuously through dashboards and reviewed by the director and the advisory board on a semi-annual basis.

6 Broader Impacts

Understanding the impact of AI across society: Large language models (LLMs) are already being rapidly integrated into consumer products, and are impacting fields outside of computer science from mathematics to medicine, and their impact on society is likely to continue to grow. However: LLMs have advanced so rapidly that civic leaders have called for a temporary pause on LLM development until academic research can catch-up [124]. The NDIF will provide the hardware, software, and training necessary for researchers to better characterize the possibilities and potential of LLMs. For example: our collaborators in psychology plan to analyze AI using tools from neuroscience, and collaborators in linguistics will analyze how aspects of knowledge are captured by LLMs. Without this vital research, it will be difficult-to-impossible for policymakers to design regulations to ensure that state-of-the-art AI systems are safe, transparent and robust. Attached letters of collaboration show scholars from a variety of states, and across fields, that attest to the broad need for NDIF.

Building national research capacity in AI: This project will have a transformational impact on the U.S. workforce, by training an intellectually diverse group of scholars to understand the potential and mitigate the harms of powerful new AI capabilities. Our planned outreach and education programs will help train the next generation of researchers to ask and answer critical questions about the capabilities and limitations of large language models, and their impact on society.

Democratic and equitable access to NDIF: As described in Section 6.1, our outreach, training and support plan is designed to democratize access to the NDIF. Our outreach plan is structured to build upon our established partnerships with Northeastern's Center for Inclusive Computing (lead by co-PI Brodley), supplemented by collaborations with the Computing Research Association (see attached letter of collaboration from Tracy Camp). Our resource allocation plan describes need-based resource grants to ensure that access to the NDIF is not simply prioritized to the largest research institutions. 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 education and 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 who are part of Northeastern's "Align" masters program, which provides a direct pathway into computing for students without a CS background. We will deploy our training curricula throughout our institution's network of campuses in Virgina, North Carolina, Florida, Maine, Massachusetts, California, and Washington. Northeastern is well-known for its experiential learning Co-Op — every student completes at least one six-month full-time internship — we have had great successes in the past recruiting students to develop software, and will continue this approach for this project.

6.1 Strengthening National AI: Outreach, Training, Virtual Community and Support

The NDIF will strengthen the US Artificial Intelligence Research & Development ecosystem. As such, we are committed to ensuring that we provide training and support to the US scientific community to ensure that the infrastructure is accessible and usable. Beyond offering "open" access to NDFI, our goal is to provide democratized and equitable access to the facility by addressing 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.

Democratic and Equitable Access 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 [125, 126]. Thus throughout all outreach we will ensure that we are reaching a diverse set of institutions, researchers and students. Co-PI Brodley, who leads the Center for Inclusive Computing (CIC) at Northeastern [127] is a nationally recognized expert in broadening participation in computing [128], and has a deep network across the country with college and university leaders of both R1 and non-R1 institutions, with a focus on reaching new PIs, and PIs in EPSCOR states and at minority serving institutions. We will recruit potential users in several ways: using popular social media channels such as twitter, through the Computing Research Association,[6] by running workshops at AI/ML conferences, and by utilizing the deep network of diverse institutions that participate in initiatives run by the Center for Inclusive Computing, which currently collaborates with 100+ universities across the country.

Developing National Expertise We will design a series of training modules to help onboard new PIs and students to the NDIF. Modules will cover topics such as: 1. How to perform reproducible inference experiments on the NDIF. 2. How to choose between different deep inference methodologies, such as representation probing, attention mapping, causal mediation analysis and parameter-efficient fine tuning. How to perform these experiments on NDIF. 3. How to deploy NDIF on your own GPU infrastructure. In the second year we will pilot an intensive in-person "bootcamp" in Boston, which will provide graduate students studying in the U.S. with hands-on access to the experts who build and maintain the infrastructure. In year three we will expand this bootcamp to six different geographic regions, leveraging Northeastern's campus network[7] and two universities partners, with a focus on cities with a major airport hub; we will run five bootcamps during the summer of 2026 in Oakland, Miami, Washington DC, Dallas and Chicago. The cost of attending the bootcamp is free[8] and will be led primarily by Northeastern PhD students with co-PI Bell and co-PI Gupta in attendance. For graduate students whose advisors do not have budget to cover the travel costs we will have a $50k fund to support travel based on need. Ad-

[6]Please see the attached letter of support from the executive director of the CRA, Tracy Camp.

[7]Northeastern offers their programs at nine global campuses, including Miami, Washington DC, Oakland, Seattle, San Jose and Portland, Maine.

[8]We will leverage the events team at Khoury for local arrangements who provide this service free of cost for Khoury faculty and the space will be provided for free.

ditionally we will offer one-day workshops using the in-person tutorials co-organized with major machine learning conferences, such as NeurIPS, ICML, ICLR, ACL, EMNLP, AAAI. We will select two conferences per 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.

Nurturing a Virtual Community Training and mentoring will continue beyond the in-person events, via a virtual community. The goal of the virtual community is to provide a space for researchers to learn more about the NDIF, and also to showcase and discuss ongoing research on the NDIF. In preparation for this proposal, we created the NDIF virtual community using the *Discord* platform. This platform enables real-time and asynchronous text communication organized by channel and thread, and provides integration audio and video chat as well. In just its first month of operations, this platform brought together 43 researchers from across the country to discuss the design and use-cases for NDIF. We will organize a virtual conference every year, providing students and researchers with a space to showcase their ongoing work and to have "ask me anything" interactions with the project team. Online, we will maintain a website with reference materials, tutorials, and examples, as well as an open-source codebase on github and we will use the public issues database as a conduit for gathering and tracking user issues. We will integrate this virtual community with our in-person training, with the goal of broadening the availability of NDIF and limiting potential barriers to its adoption.

6.2 Undergraduate Education

We are committed to ensuring that undergraduates at Northeastern and beyond benefit from the proposed infrastructure. 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 Northeastern (e.g., Machine Learning I and II, NLP, and Practical Neural Networks). Bau and 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.

Importantly, once developed, we will make these materials—which will use the hosted API developed and instantiated under this project—available to faculty at other institutions, scaling the impact by enabling undergraduates in CS across the U.S. to gain hands-on experience analyzing and working with the internals of massive language models, which increasingly dominating the AI landscape. Note that such exercises are not currently possible at the vast majority of institutions given the resources required to run such models. And even if students are willing and able to pay for access via a commercial API, they would not be able to access model internals in a granular way, in turn severely limiting the kinds of analysis possible. As discussed in Section 6.1 we will ensure that we are supporting universities/colleges across the country with a particular focus on outreach to minority-serving institutions, women's colleges, HSIs, and HBCUs.

7 Institutional Commitment to Inclusion

Khoury College of Computer Sciences is a leader in broadening participation in Computer Science (CS). Khoury is home to the Center for Inclusive Computing (CIC) [127]), which aims to increase the representation of women of all races and ethnicities majoring in CS across the U.S. The CIC works with over 100+ institutions across the country to remove institutional barriers to students discovering and persisting in computing. Under co-PI Brodley's leadership, Khoury piloted and scaled the Align MS in CS program [129, 130], 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 are 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 [131], a networked community of 23 institutions who are now offering the MS in CS for non-majors. Khoury also has a verified college-wide broadening participation in computing plan [132].

8 Divestment

Northeastern Research Computing will maintain NDIF hardware for their lifetime at no direct cost. This includes the cost of safely disposing of computing equipment as needed. In the event the project becomes insolvent, Research Computing will erase all disk storage on NDIF and repurpose the hardware for other research. Thus, a full decommissioning will not incur additional costs.

However, we our aim is to keep NDIF operating for as long as possible beyond the expiry of this proposal. We hope to build a community of expertise on the open-source NDIF software. This community of experts will include not just the PIs and NDIF stuff, but also students and researchers across a broad range of U.S. colleges and universities. With community-driven support for yet-to-be-released models and inference technology, we should be able to keep NDIF up-to-date and relevant for researchers.

8.1 Future-proofing the NDIF infrastructure investment

We recognize that large-scale machine learning is a rapidly evolving field, and we are committed to designing the NDIF to be future-proof. To maximize the number of years for which researchers will be able to utilize the facility to solve critical research problems in the face of inevitable future changes and innovation in machine learning, our plans incorporate several strategies.

First, our technical design will be built upon foundational, modular methods [133] that have been the backbone of machine learning architectures since 1990. Deep learning frameworks such as Pytorch have used a similar strategy, and we will build upon those specific technologies and exploit the same insight: even as large-scale machine learning architectures evolve, properly designed modular methods are timeless and will continue to apply.

Second: in our operational design, we will architect the system to be able to execute research workloads on a variety of computation platforms, not just our own cluster, so that research users can exploit or send peak load to computational facilities available elsewhere if computation capacity needs exceed our own cluster. Platforms we are envisioning include commercial cloud providers [66, 134–136] as well as nonprofit clusters [65, 137] and the future NAIRR [13].

Third: during and after development, our scientific advisory board and our technical change committee will regularly review the set of architectures, interfaces, and features that we support in the face of current research, to ensure that we are supporting work on specific architectures and capabilities that are most relevant in to current and future research questions. Our design and deployment process also includes continuous community feedback and frequent design reviews. Our development process is designed to adapt the design of the system if there are significant technology changes during development.

Finally, our development team will focus on building an open-source community, not just a static software offering, so that the NDIF will have the ability to continue to evolve after the facility is established. We will conduct our development in the open and actively engage open-source participation, using public source code repositories, public issue-tracking systems, and public online discussion forums. Our project will create a software architecture and organizational structure that is intended adapt to technology evolution. Through all these steps, we will ensure that the NDIF remains a valuable resource for researchers well into the future.

9 International Collaborators

Our project does not involve international collaboration. No-fee usage of the facility will be provided to US educational users only. When the service is established, international researchers can apply to join the facility as paid NDIF partners.

10 Results of Prior NSF Support

PI Bau is a late-career academic with substantial industry experience, and this is his first NSF grant proposal. He has recruited a team with a strong track record with the NSF that includes Co-PI Brodley, former Dean of Khoury College, as well as several other collaborating PIs. Professor Bau previously worked at Google, where he created and managed the Google Talk and Hangouts team and led the Boston Google Image Search ranking team. He has a track record managing projects to develop large-scale online platforms with global reach and real-world impact, processing exabytes of data and answering billions of user queries each day.

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. One award is #2137907: BPC-DP: Distributed Research Apprenticeships for Master's (DREAM), (2021-2023) 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.

Co-PI Wallace is PI multiple active NSF awards; of these the most related to the current proposal is "RI: Medium: Learning Disentangled Representations for Text to Aid Interpretability and Transfer" (NSF 1901117, $999,990.00, 2019-2023). **Intellectual Merit:** This project endeavors to develop neural networks that yield *disentangled* representations, i.e., embeddings that 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 [85, 98, 100, 105–107, 138]. **Broader Impact:** The primary focus of this work is to realize varieties of transparency via disentanglement; this technical focus 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). PI Bell's work on this project has been focused on detecting flaky tests [117], understanding flaky tests [139–141], and making CI builds faster [142]. **Broader impact:** PI Bell's work on CI has resulted in several significant technology transfers to popular the open-source projects Apache Maven [142] and Pitest [140]. New educational materials for CI have been developed and shared under the creative commons license [143, 144]. PI Bell has mentored six undergraduate, two masters and three PhD students on this project.

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 [112, 145–148]. Wasm/k [146] implements continuations for WebAssembly, a growing platform for serverless computing. **Broader Impact**: PI Guha is standardizing WebAssembly effect, informed by Wasm/k.

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