Creating Intelligent Cyberinfrastructure for Democratizing AI: Overview of the Activities at the NSF-AI Institute ICICLE

Talk at Chinese Academy of Sciences, Beijing, China (Nov. 2023)

by

http://icicle.ai

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Credits to all ICICLE Team Members!!

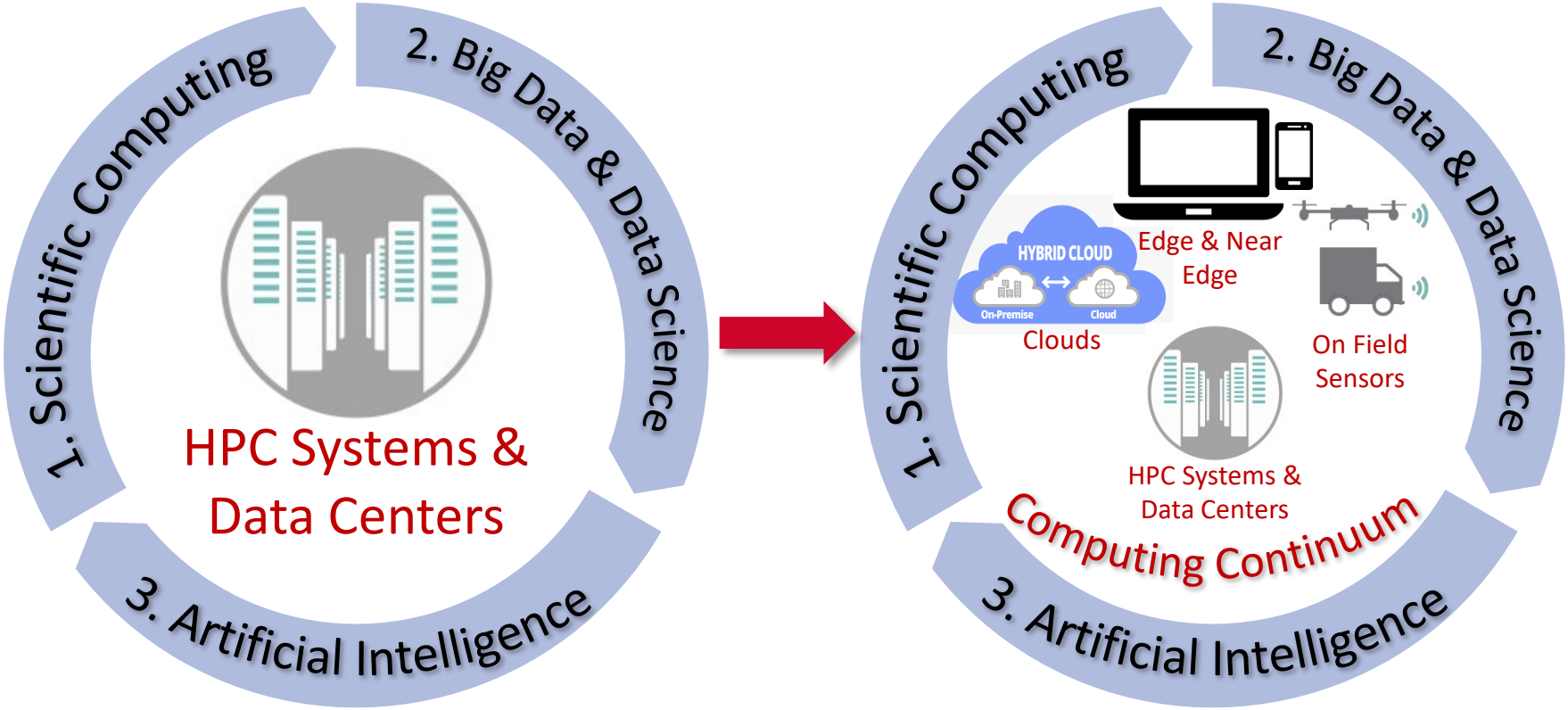
Outline

- **ICICLE Vision and Goals**
- Research Challenges Addressed
- Highlights of Selected Accomplishments
- How to Get Engaged?
- Conclusions

Computing has been evolving over the last three decades with multiple **phases:**

- Phase 1 (1975-): Scientific Computing/HPC
- Phase 2 (2000-): HPC + Big Data Analytics
- Phase 3: (2010-): HPC + AI (Machine Learning/Deep Learning)

Emergence of the Computing Continuum



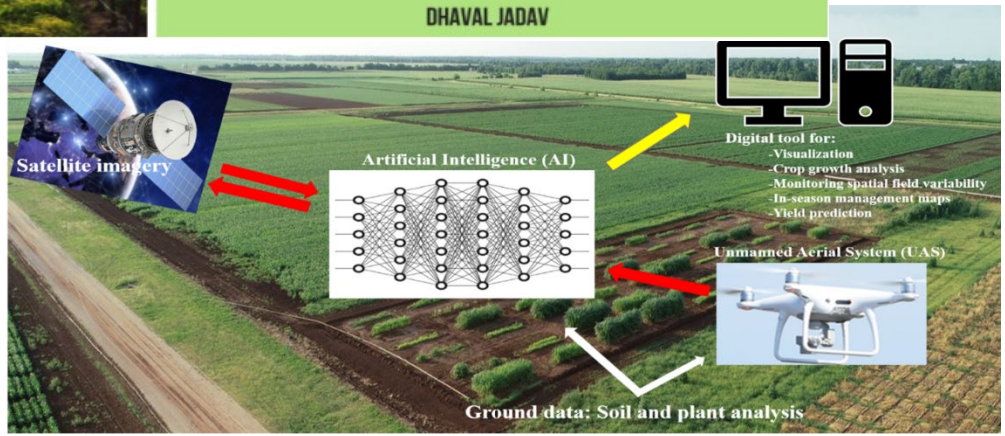
Societal Challenge (Example #1): Agriculture

- **Food security/sustainability in 2050**
  - 9.8B people, climate; 0.5x arable land per cap vs 1985
  - Wide gains in crop management needed (typical yields fall 3X below best practice)

- **Sustainable agricultural workforce**
  - The next generation of agriculture professionals will include engineers, computer scientists, data scientists

- **Democratization of digital agriculture capabilities**
  - Autonomous unmanned aerial vehicles, self-driving tractors and sprayers, fertilizer and seed recommendations
  - Big and small farms, staple and specialty crops, underrepresented communities
  - Privacy and ethical considerations

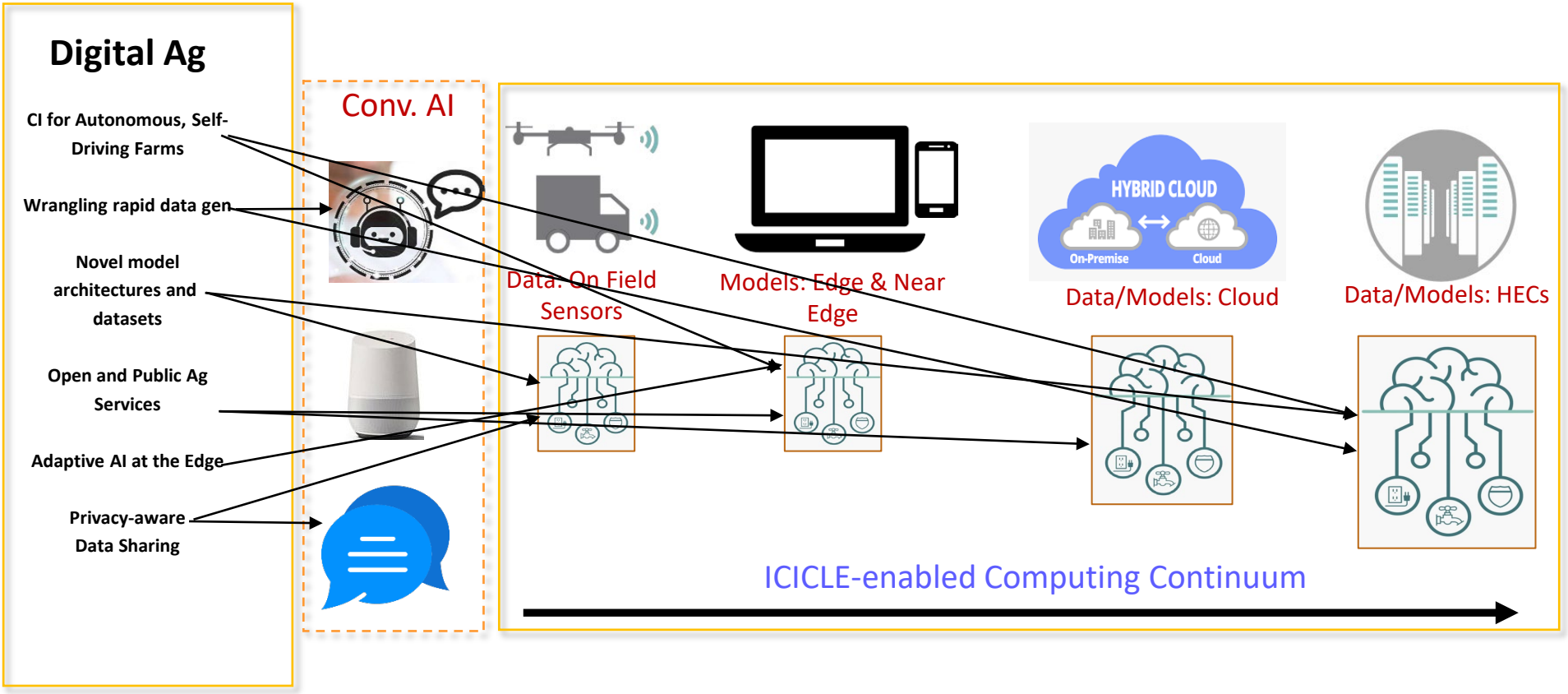
AI-Driven Digital Agriculture



https://ccag.tamu.edu/research-project/digital-agriculture/

https://medium.datadriveninvestor.com/artificial-intelligence-in-agriculture-62f71f8f6ae6

Challenges in Designing AI-Driven CI for Digital Agriculture in Computing Continuum



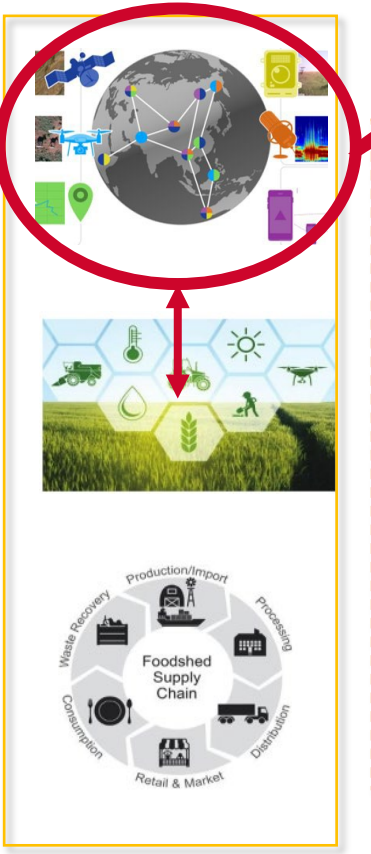
Societal Challenge (Example #2): Animal Ecology

- **Basic science:** The focus of Animal Ecology is understanding the functioning and behavior of animals individually and in groups *in the context of environment* and evolution.

- **Science + translational:**
  - Monitoring, understanding, and protecting biodiversity of the planet
  - Monitoring and understanding the impact of changing habitats on animals that live in them

- **Translational:** biodiversity conservation and mitigating the impact of climate change

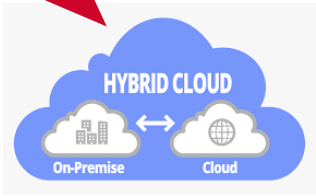
Challenges in Designing AI-Driven CI for Animal Ecology in Computing Continuum



Conv. AI

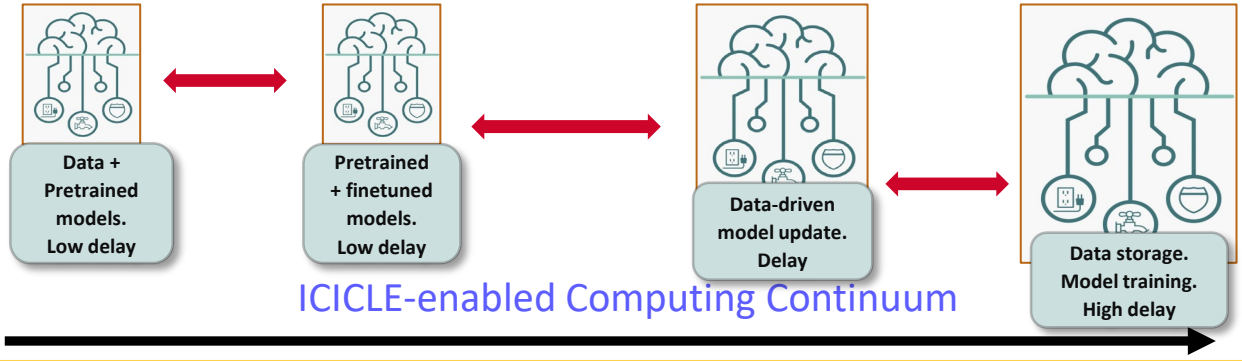
Data: On Field Sensors

Models: Edge & Near Edge



Data/Models: Cloud

Data/Models: HECs



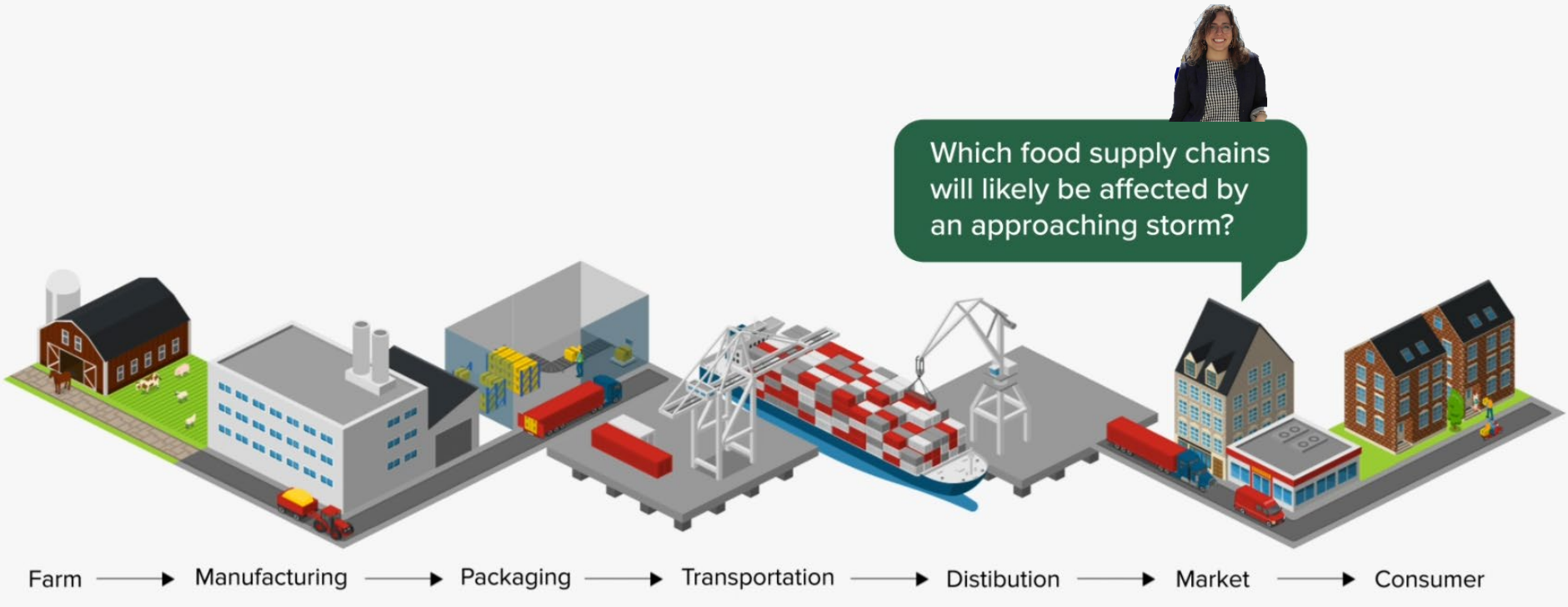
ICICLE-enabled Computing Continuum

Resource+delay/model accuracy+analysis scope TRADEOFF

Societal Challenge (Example #3): Smart Foodsheds

- **Food Supply Chain Vulnerabilities**
  - Concentration contributes to bottlenecks, lack of resilience to disruptions
- **High Food Insecurity**
  - Supply chain decisions fail to account for impacts on food access, cost, availability
- **Food Waste**
  - Inefficiencies in food supply chains and food systems lead to 30-40% waste
- **Negative Environmental Footprint**
  - Farming and food system has major impacts on environment
- **Holistic Food Systems Planning is Difficult**
  - Data is difficult to access, not coordinated across sectors or food supply chain actors

AI-Driven Foodshed Supply Chain Management?



Challenges in Designing AI-Driven CI for Smart Foodsheds in Computing Continuum

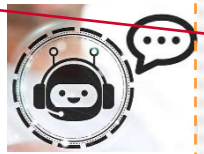
Smart Foodsheds

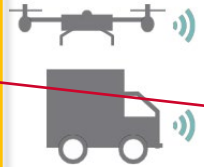
Diverse data sources **database federation**

Heterogenous food systems and actors **Conversation agents and knowledge graph**

Food system planning **Easy-to-use intelligent visual analytics**

Conv. AI





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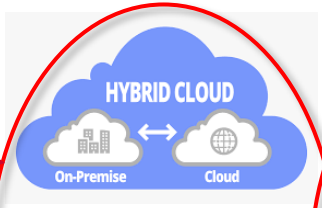

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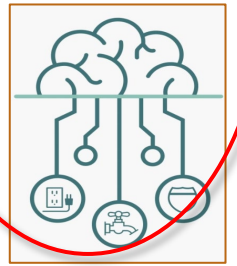


ICICLE-enabled Computing Continuum

How AI can Help the Users of these Science Cases?

For the three use-inspired science cases:

- Massive and ever-growing gap between AI and its accessibility to the users
- Existing AI applications are developed largely ad-hoc and lack coherent, standardized, modular, and reusable infrastructure
- Successful AI solution(s) for one use case rarely generalize to other use cases, or even the same use case even with slightly different context.

CI's complexity to deploy AI impedes research discoveries and innovations!

Many more examples

- Smart Cities
- Smart Manufacturing
- Smart Transportation
- Real-time Surveillance
- Computational Medicine (Pathology, Radiology, ..)

Broad Challenge

Designing the next-generation intelligent cyberinfrastructure for a computing continuum with heterogenous resources that is usable in a plug-and-play manner by stakeholders to solve societal challenges?

The ICICLE Overview Video

The Video is available from

https://youtu.be/gNFk5tDTtoU

The Vision

A **national infrastructure** that will:

- Catalyze **foundational AI/CI** and transform application domains
- **Democratize AI** through **integrated plug-and-play AI**
- **Transparent and trustworthy** infrastructure for AI-enabled future
- Address **societal problems** (agriculture, conservation, food insecurity) **globally**
- Grow **new generations of workforce** and incubate **sustainable and inclusive** communities

Objectives: Intelligent CyberInfrastructure for Computing Continuum

Use Inspired Science Domains

Digital Agriculture

Smart Foodsheds

Animal Ecology

ICICLE: Intelligent CyberInfrastructure with Computational Learning in the Environment

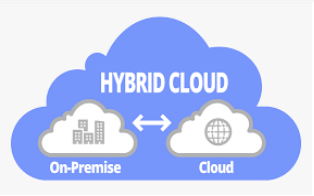
Systems AI Foundational Research for CI

Intelligent Cyber Infrastructure

CI for AI | **AI for "CI for AI"**

On Field Sensors

Edge & Near Edge

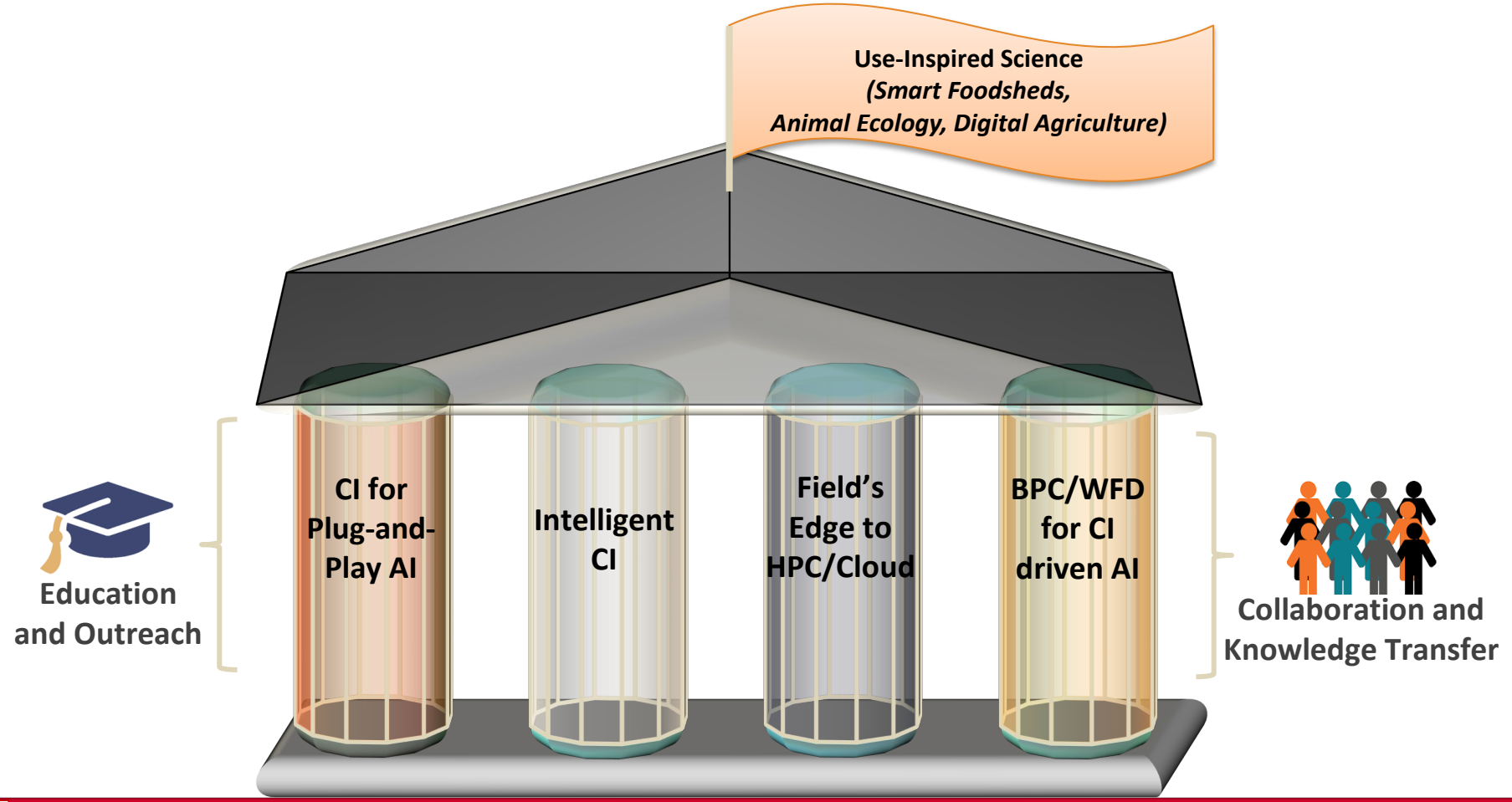


Clouds

HPC Systems & Data Centers

Emerging Computing Continuum

ICICLE As A Whole



Participation:
14 Organizations, 33 faculty, 41 staff, (58 PhD, 16 MS, 16 undergrad, 6 K-12) students & many Collaborators

Govt. Agencies & National Labs

Lawrence Livermore National Laboratory
U.S. Fish & Wildlife Service
Brookhaven National Laboratory
Fermilab

International

Max-Planck-Gesellschaft
University of Stuttgart Germany

Research Institutes

national center for women & information technology
MolSSI
SGCI Science Gateways Community Institute
TRUSTED CI The NSF Cybersecurity Center of Excellence
ECEP
CAHSI Computing Alliance of Hispanic-Serving Institutions
SCEC An NSF+USGS Center
NSF NEON Operated by Battelle
Jetstream

Industry

CNH Industrial
ADC
WildMe
Microsoft
Farm 2 Facts
The Findings Group, LLC Research & Evaluation

NSF AI Institutes

AIFS AI Institute Food Systems

Hospitals & Universities

Nationwide Children's
University of North Carolina at Chapel Hill
Princeton

Collaboration: ICICLE and the Technology Innovation Hub (TIH) at the Indian Institute of Technology Bombay (IIT-B), India

Digital Agriculture



This research collaboration will contribute novel design paradigms for context-adaptive CI and aims to develop next-generation CI for *Digital Agriculture* including AI and machine learning methods targeting 3 core areas.

Crop Health Modeling

- Sense crop health and level context to predict crop yield
- Detect stressors and diseases for geographically diverse crops
- Apply remedies with little human intervention via Internet of Things (IoT) and sensor systems

Aerial Crop Scouting

- CI for fully autonomous aerial systems
- Simplify deployment of UAV in real fields to capture common crop health conditions
- Provide accurate maps that yield valuable insights for crop management

Privacy-Preserving Data Exchange

Create secure, trustworthy, and privacy-preserving platforms that connect farmers and allow them to share information and resources safely.

Building upon the existing ICICLE infrastructure, CI and AI capabilities, researchers will leverage contextual conditions in India for *Digital Agriculture* that differ from the United States to (1) expose brittle CI components, (2) make AI4CI more robust and expansive in the long-term, (3) devise principles that yield context-aware CI

External Advisory Board (EAB)

Ewa Deelman
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University of Minnesota
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Use-Inspired Science, Industry

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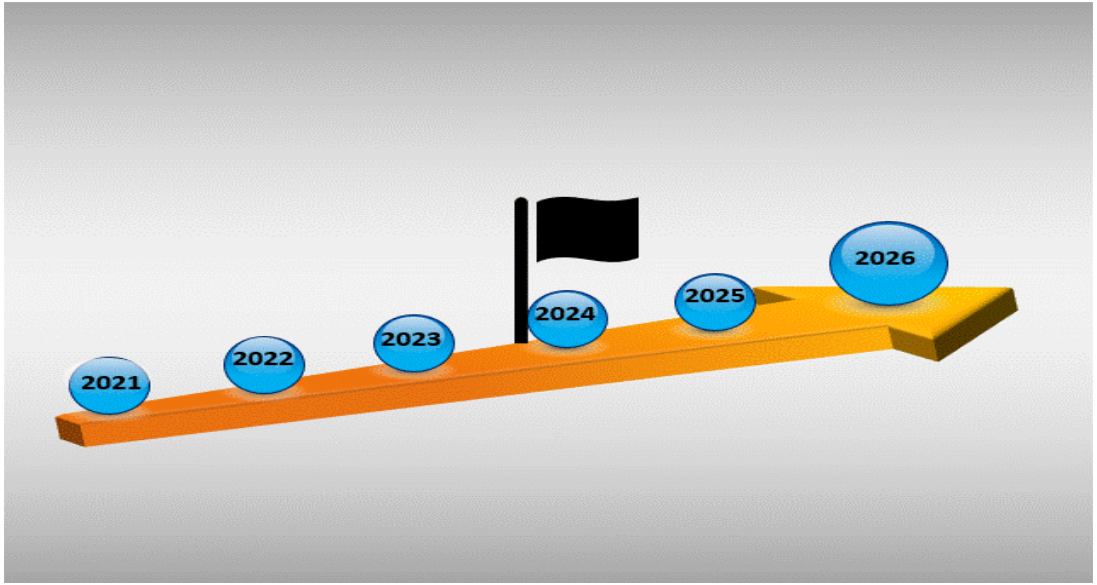
Argonne National Laboratory
WFD/BPC, Lab/HPC

Tiffani Williams
Univ. of Illinois, Urbana-Champaign
WFD/BPC, Academia

Luke Zettlemoyer
Meta and Univ. of Washington
Artificial Intelligence, Industry

Timeline

- Started on Nov 1, 2021
- Finishing 24 months of the project



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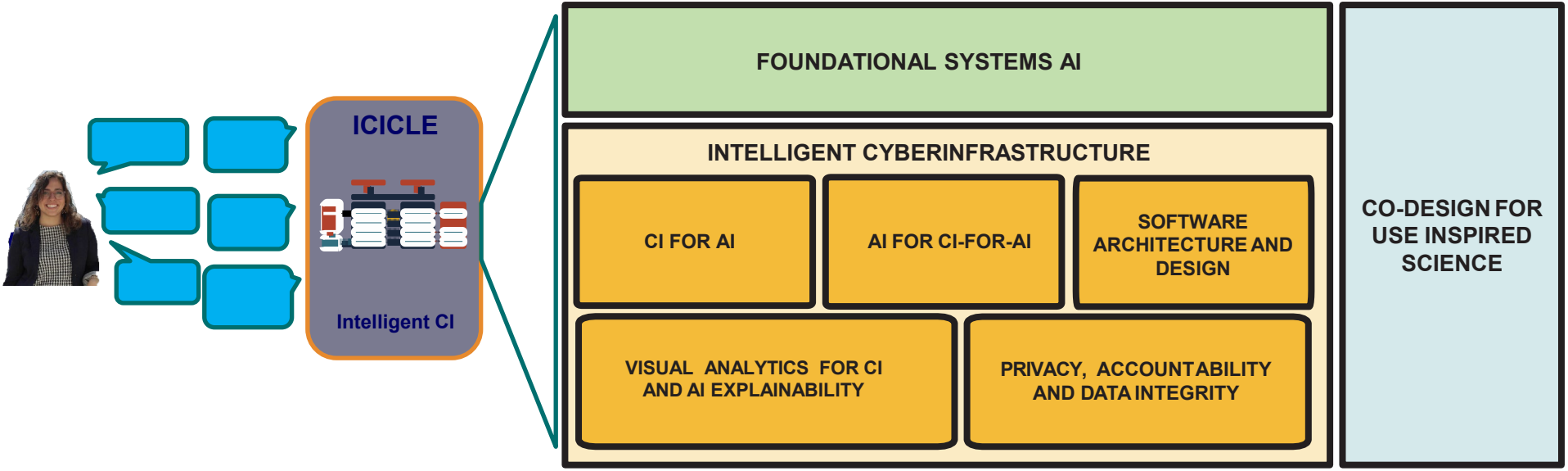
- **Research Challenges being Addressed**
- Selected Accomplishment Highlights
- How to Get Engaged?
- Conclusions

Research Plan: Overall Vision



Thrust: Foundational Systems AI

Components address CI complexity and heterogeneity for plug-and-play

Knowledge Graphs

- Multimodal KG to encode & reason rich data modalities (e.g., camera trap)
- Auto construction
- Interplay with LLM and knowledge-based QA

Model Commons

- MINT to support ICICLE use cases, KG, and models
- Precise profiling
- Flex composition
- Versioning and provenance

Adaptive AI

- Context-aware
- Efficient update
- User-friendly adaptation process
- Adaptation of foundation models, conversational AI

Federated Learning

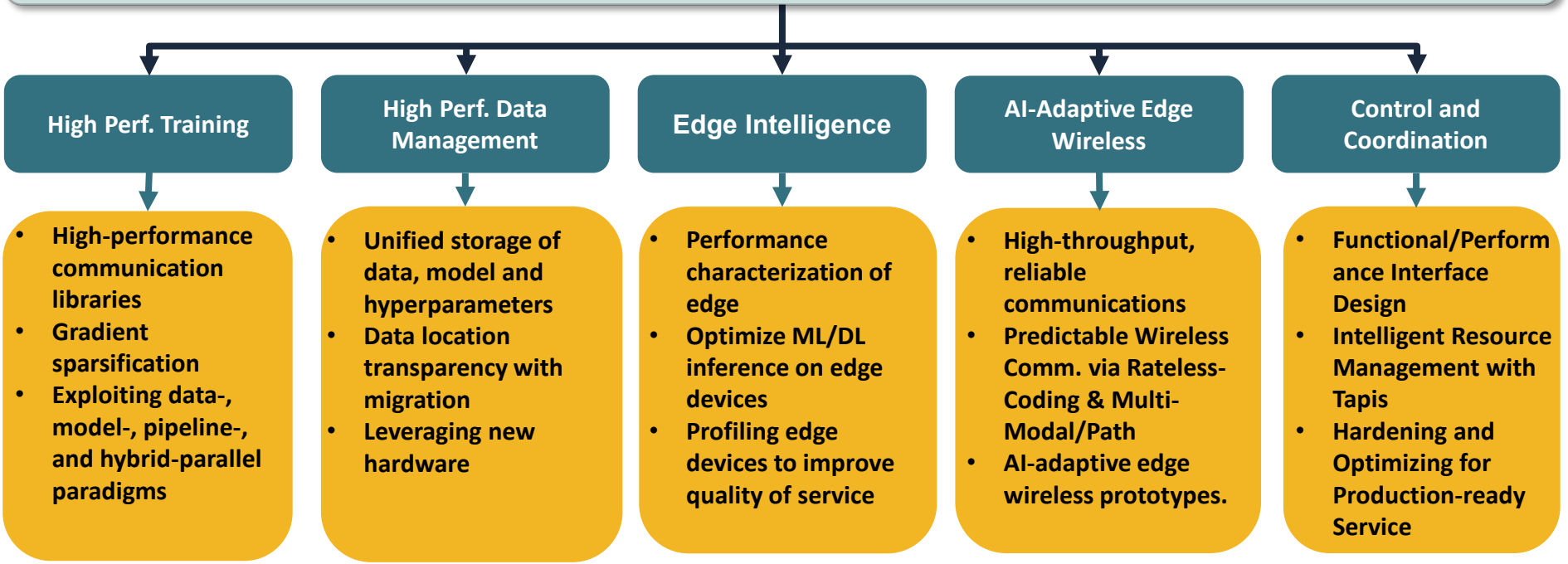
- Heterogeneity
- Context-aware
- Privacy-preserving and robustness
- Going beyond classification (GNN, foundation models)

Conversational AI

- KG- and model-commons-aware
- LLM-powered
- Grounding LLMs to the context
- Hallucination reduction
- Complex reasoning

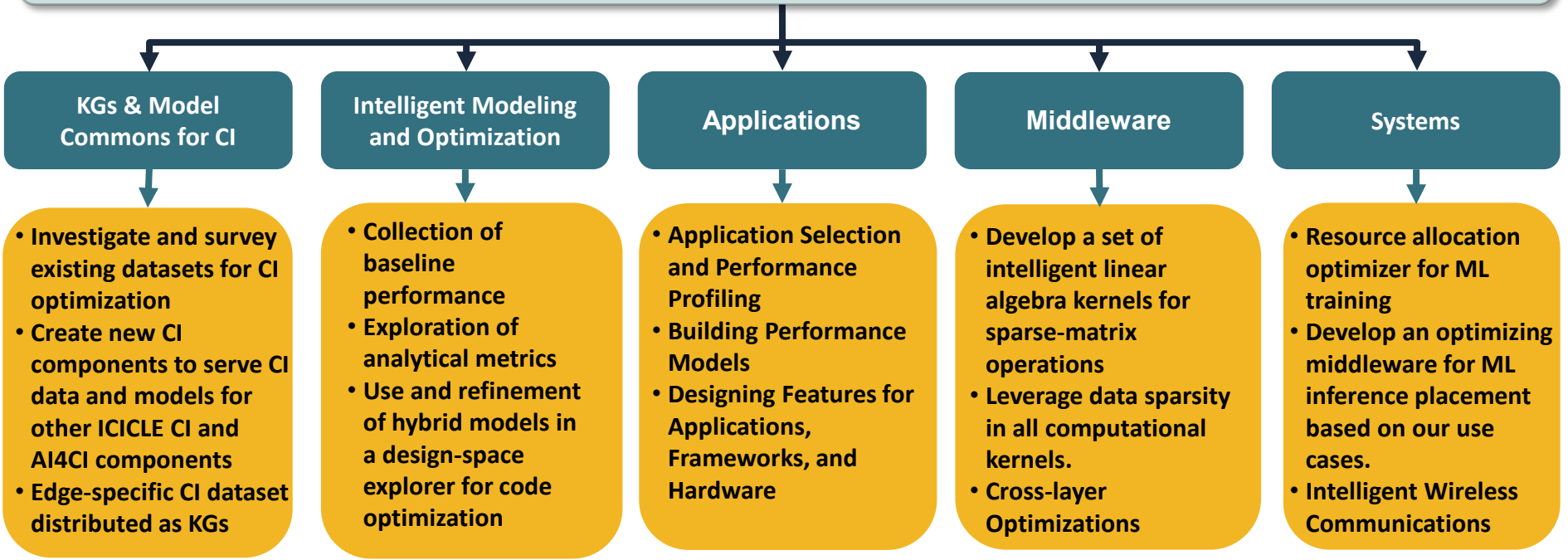
Thrust: CI4AI

Provides necessary CI to deploy AI throughout computing continuum and make it plug-and-play!



Thrust: AI4CI

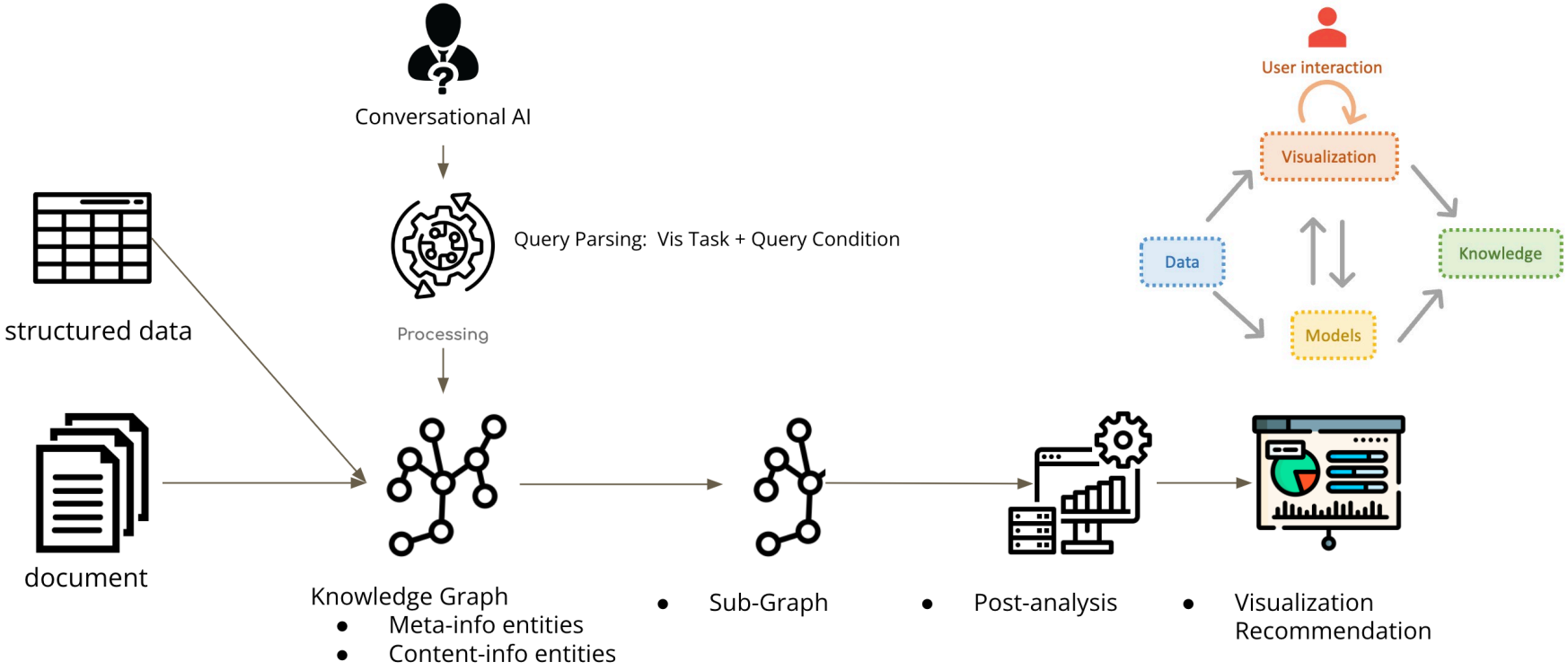
Enhances CI with AI for adaptive and field-optimized machine learning!



Thrust: Privacy, Accountability and Data Integrity (PADI)

- PADI contributes to
  - ICICLE vision as *transparent and trustworthy* infrastructure for AI-enabled future
  - An ethically aligned infrastructure and workforce through an *AI ethics framework*
- PADI advances both technical and non-technical innovations and best practices that collectively contribute to a trusted environment
  - e.g., where stakeholders (farmers, industry partners, etc.) are comfortable contributing data and AI models for ICICLE AI research (and more broadly for AI research).
- PADI addresses both research questions and issues of practice (project norms and practice)

Thrust: Visual Analytics



Co-Designing with use-inspired domains

Conv. AI

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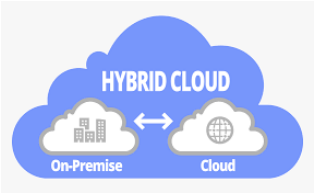

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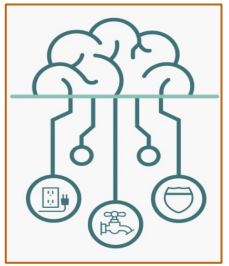
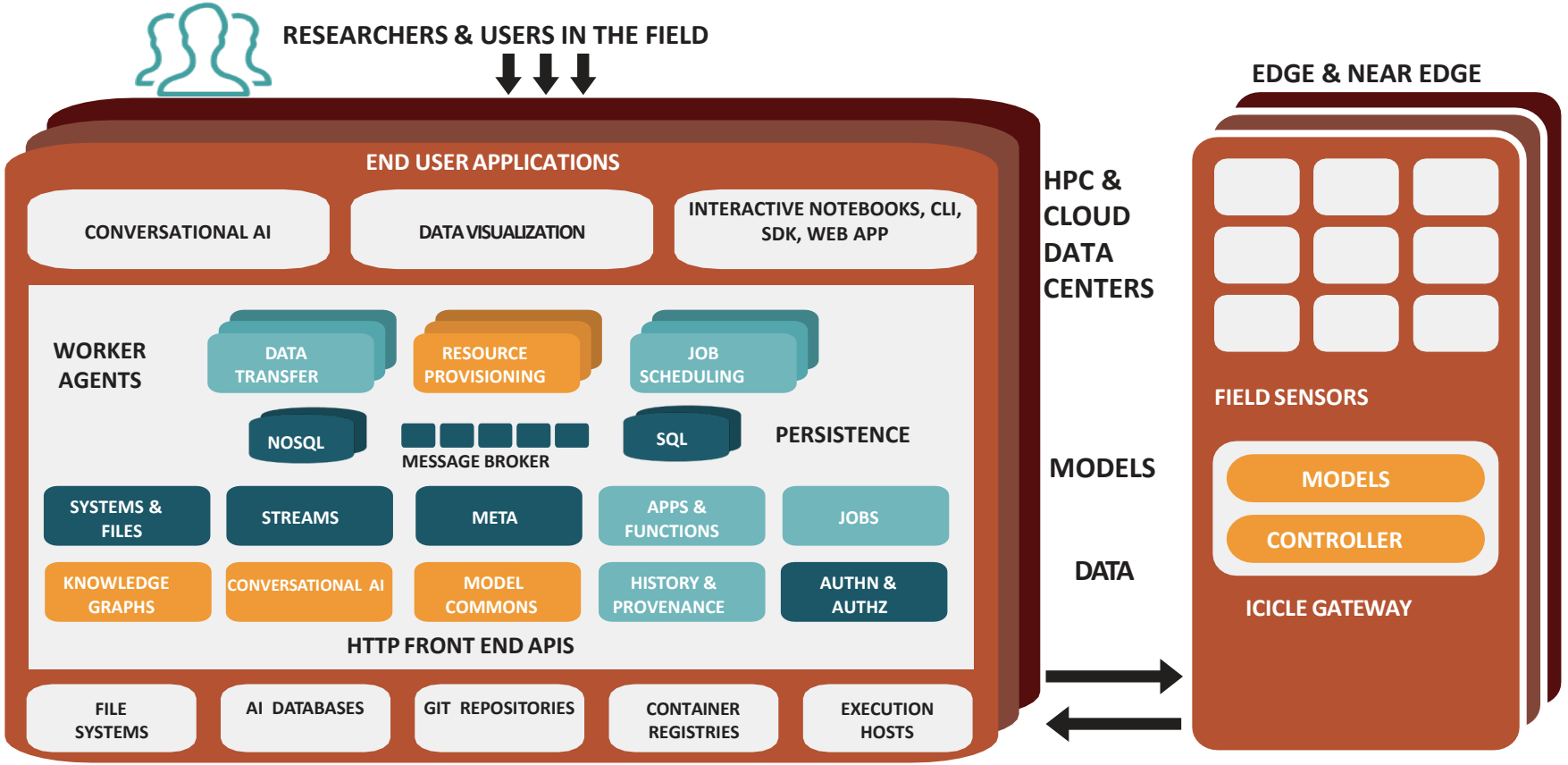


ICICLE-enabled Computing Continuum

The Deliverable: The ICICLE Software Stack

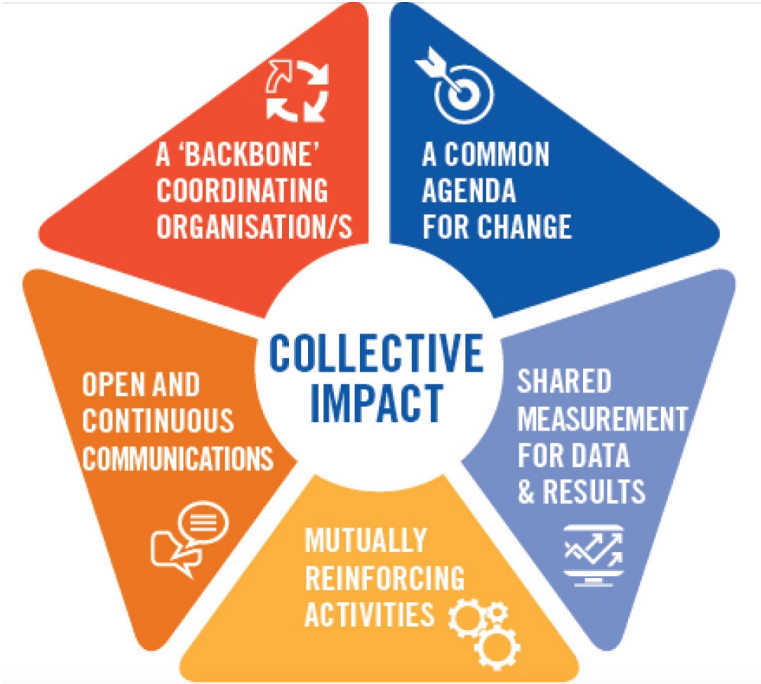


Broader Impacts Backbone Network (BIBN)

BIBN is a consortium with the goal of democratizing AI!

Oversees activities towards broader impacts and engagement:

- Diversity Equity and Inclusion (DEI)
- Broaden Participation in Computing (BPC)
- Workforce Development (WFD)
- Collaboration and Knowledge Transfer (CKT)



Outline

- ICICLE Vision and Goals
- Research Challenges being Addressed
- **Selected Accomplishment Highlights**
  - **CI/Software Released**
  - **Digital Agriculture (demo)**
  - **Smart Foodsheds (demo)**
  - **Grocery Store Closure (demo)**
  - **AI4CI**
  - **BIBN**
- How to Get Engaged?
- Conclusions

CI/Software Components Released (so far)

2023.04 Release (04/30/23)

- **AI4CI**
  - HPC Application Runtime Predictor (HARP) v1.0
  - Intelligent Sparse Library (iSpLib) v1.0
- **Software and Reference Architecture**
  - Base ICICLE Tapis Software v1.3.0
  - Event Engine v0.2.0
  - Hello ICICLE Authentication Clients v0.0.1
  - Tapis Pods Service v1.3.0
  - CI Components Catalog v0.1.0
- **Animal Ecology**
  - Camera-Traps Edge Simulator v0.3.0
- **Digital Agriculture**
  - SoftwarePilot v1.2.5
- **Smart Foodsheds**
  - Persons-Projects-Organizations-Datasets (PPOD) Schema v0.9.1
  - Smart Foodsheds Visual Analytics (VA) Dashboard v0.1

2023.06 Release (06/30/23)

- **AI Foundations**
  - ICICLE Foodshed Parser v0.1
  - Species Classification using Multimodal Heterogeneous Context v0.1.0
  - Region2vec v1.0
- **Software and Reference Architecture**
  - Tapis Federated Authentication Service v1.3.4
  - ICICONSOLE v0.0.10
  - TapisCL-ICICLE v0.1.4
  - Tapis Pods Service v1.3.2
- **Animal Ecology**
  - Camera-Traps Edge Simulator v0.3.1
- **Digital Agriculture**
  - ICICLE Digital Agriculture Hub v1.0
  - Far-Edge Edge Simulator v1.0
  - In-Field Helper for Crop Scouts v1.0
- **Smart Foodsheds**
  - Persons-Projects-Organizations-Datasets_California (PPOD_CA) Knowledge Graph v23.06
  - Kroger Store Closure v0.1
  - Smart Foodsheds Visual Analytics (VA) Dashboard v0.2

https://icicle.osu.edu/cyberinfrastructure/software

CI/Software Components Released (so far)

2023.10 Release (10/06/23)

- **AI4CI**
  - HPC Application Runtime Predictor (HARP) v2.0
  - High Performance Computing Applications Dataset v1.0
- **Software and Reference Architecture**
  - iciflaskn v1.0
  - ICICONSOLE v0.8.0
  - TapisCL-ICICLE v1.0.11
- **Animal Ecology**
  - Camera-Traps Edge Simulator v0.3.2
- **Smart Foodsheds**
  - Smart Foodsheds Visual Analytics (VA) Dashboard v0.3

https://icicle.osu.edu/cyberinfrastructure/software

Digital Agriculture

What does CI for digital agriculture look like?

How to build CI that connects a wide range of digital agriculture stakeholders?

Why use-inspired CI will be transformative?

ICICLE Use-Inspired Science: Digital Agriculture

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Food, Agriculture and Biological Eng.

Christopher Stewart
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Co-Leads

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Digital Agriculture Hub and Use-Inspired Technologies

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Hari Subramoni

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Cyberinfrastructure for AI-Driven Digital Agriculture

Erman Ayday
Case Western

Beth Plale
Indiana University

Privacy-aware, Explainable AI, & Democratization

Alfonso Morales
University of Wisconsin

Stakeholder Engagement

Digital Agriculture – Crop Management

Digital Agriculture will transform crop management by:

(1) sensing environmental conditions
(2) characterizing crop health at fine granularities
(3) autonomously delivering cost-effective treatments

Stakeholders include farmers and biologists—traditional agriculture professionals—**and** data scientists, machine learning experts, engineers, and HPC professionals

ICICLE seeks to develop CI needed for all stakeholders to create, share, and process agricultural data effectively and efficiently

Image from Molly Caren Agricultural Center, OSU's 2100 -acre facility

In this context, AI will drive improvements in:

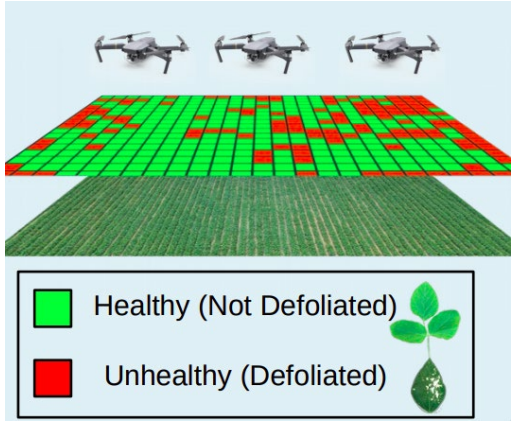
(1) Autonomous, self-driving farms
(2) Methods to wrangle the rapid growth of agricultural data
(3) Data-driven and context-aware agricultural insights
(4) Context-aware management and differential privacy
(5) Managing open & democratized digital agriculture services

Digital Agriculture: Aerial Crop Scouting

- **Aerial Crop Scouting:** In this workload, we seek to create *heat maps* that describe crop health for a field
  - *Inform* self-driving tractors and sprayers to reduce the application of pesticide and fertilizer
  - *Predict* crop yields for harvest and market timing
  - *Identify* trends across farms, such as the introduction of resistant weeds

- **Technology:** Unmanned aerial vehicles (UAV) capture high resolution images
  - Flying low (15 ft above ground): 1 pixel -> mm

- **Transformative:** At mm-granularity, stakeholders can detect biological phenomena invisible to satellites
  - Soybean leaf defoliation caused by Japanese beetle



Courtesy of LaRue Farms Inc.

Demo: Semi-Supervised Learning

The Video is available from

https://youtu.be/EYzAZWGvyJI

Demo: Cloud-to-Edge Middleware

The Video is available from

https://youtu.be/M6o0NVQXny0

Smart Foodsheds

The Challenges

- Food system lacks resilience (highlighted by the pandemic)
- Food system actors are diverse, work in silos
- Access to data is difficult as is reconciling across data sources
- Need a common framework to organize, share, visualize, and deploy datasets and workflows

The Strategies

- Develop relationships between ICICLE and private partners to empower stakeholders to access, interpret, and utilize food systems processes, trends, and outcomes
- Use knowledge graphs to link domain knowledge of the environment, agriculture, food, diet, and health
- Develop PPOD, a schema that describes the attributes and relationships between **Persons, Projects, Organizations and Datasets** and instantiate it with real data from California and Ohio as a first use case.

Interactive Knowledge Learning & Environment (IKLE) for Smart Foodshed


Yamei Tu


Xiaoqi Wang


Rui Qiu


Han-Wei Shen

The Ohio State University


Patrick R Huber


Allan D Hollander

University of California Davis


Matthew Lange

International Center for Food Ontology Operability Data and Semantics (IC-FOODS)


Michelle Miller


Jinmeng Rao


Song Gao


Alfonso Morales

University of Wisconsin-Madison


Christian R Garcia


Joe Stubbs

The University of Texas at Austin Texas Advanced Computing Center

Demo : Smart Foodsheds + Visual Analytics (IKLE)

The Video is available from

https :// youtu.be/ WEFDcKTl3UY

GROCERY STORE CLOSURE & COMMUNITY HEALTH

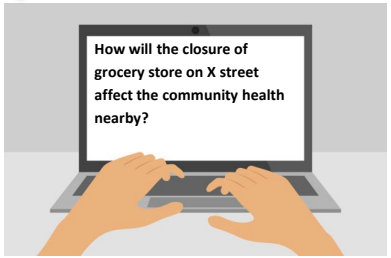
Pain points

- In public health and food systems, computer models are not used or have limited impact because decision-makers are not able to access them in a practical and timely manner.

SCENARIO

A food retail company announces plans to **close a grocery store** in a Columbus, Ohio neighborhood with **very high % of food-insecure households**.

Now the health commissioner wants to know how the grocery store closure will affect community health so they can lobby the food retail company to not close the grocery store or set up emergency food supply to reduce the impact on community health.



Our Solution (and use case in ICICLE)

A conversational AI-enabled web interface that allows decision-makers to run "What if?" scenarios based on an agent-based model for food insecurity.

Use Case

Objective: Help food system leaders quickly evaluate the impact of a food store closure on household food insecurity

Significance: Improving access to community-informed computational models empowers communities to use models to make better decision involving complex systems, such as the local foodshed.

Grocery Store Closure Team







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Demo: GROCERY STORE CLOSURE & COMMUNITY HEALTH

The Video is available from

https :/ / youtu.be/ GYjMeaE74s k

AI4CI: HARP – HPC Application Runtime Predictor

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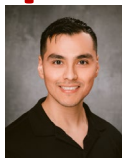

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n-tasks-per-node	Walltime (mins)	Cost Per job ($)
10	8.5954	0.01719
14	8.5768	0.01886
20	8.5852	0.02189
28	8.5931	0.02492

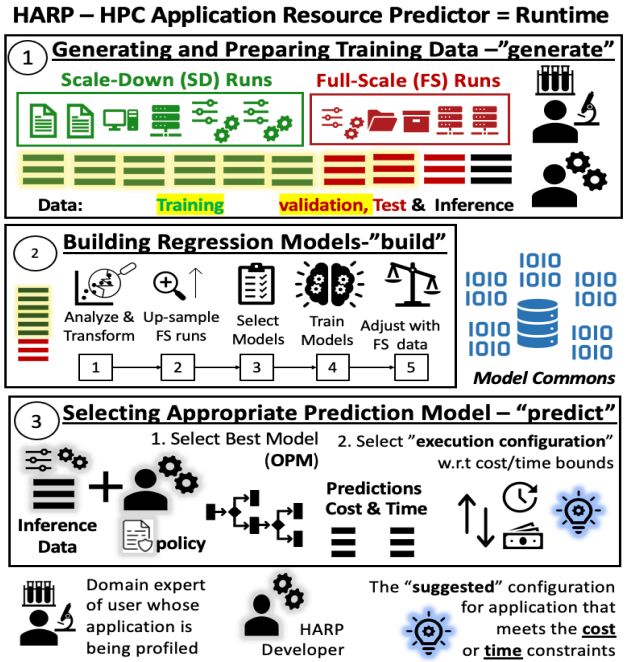
Cost ↓ ~30%

Goal

Estimating the resource requirements to execute an application on shared cyber infrastructures to aid recommendation systems or smart job allocations.

Accomplishments

- **Understanding the allocation behavior of different users against different systems and ways for optimizing the allocations.**
- **Establishing an end-to-end application-independent framework called HARP (HPC Application Runtime Prediction) that can emulate the application executions, profile them, and estimate the resource requirements against targeted environments with cost/time constraints.**



Broader Impact Backbone Network (BIBN)

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ICICLE NextGens Community Leader

Rajiv Ramnath

The Ohio State University

Mary Thomas

San Diego Super Computing Center

Selected Accomplishments from BIBN

- BPC
  - Inclusive environments initiative: **ICICLE NextGens** group, **ICICLE Code of Conduct**
  - Building awareness: bi-weekly **Ally tips (bias);** AI Ethics tips purposed for Indiana Univ **K-12 summer camp**
- WFD
  - **Hello ICICLE:** clients (Notebooks, command line, python, Web client) for testing software
  - Summer 2023 launch of **ICICLE AI Ethics tips** series of 6 videos
  - Consolidation and organization of **ICICLE Publication and Training Resources** (with WFD and HelloICICLE)
- KT
  - ICICLE Seminar Series
  - **Partnership Agreements** for stakeholders to engage with ICICLE. (Students, Academic Scholars, Organizations, Industry Sponsored, and Stakeholder Roundtable)
  - Engaging stakeholders, including through 2023 class of 5 **ICICLE Educational Fellows**

https://icicle.osu.edu/knowledge-transfer/youtube-channel

Outline

- ICICLE Vision and Goals
- Research Challenges being Addressed
- Selected Accomplishment Highlights
- **How to Get Engaged?**
- Conclusions

Multiple Levels of Collaboration and Engagement

- Using the Released Software/CI components
  - Available at https://icicle.osu.edu/cyberinfrastructure/software
  - Get engaged as a member in the Stakeholder Roundtable (more details below)
- Become a part of ICICLE (multiple options)
  - Student Associate
  - Visiting Research Fellow
  - Academic Collaborator
  - Industry Partner
  - Stakeholder Roundtable Member
  - More details at: https://icicle.osu.edu/engagement/join-us
- Join the ICICLE mailing lists (https://icicle.osu.edu/engagement/mailing-lists)
  - icicle-announce
  - icicle-discuss

Outline

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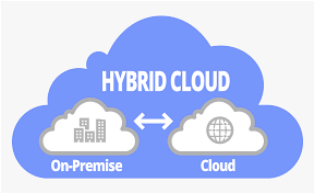
- **Conclusions**

Designing Next-Generation CI through Co-Designing with Use-inspired Domains

Conv. AI

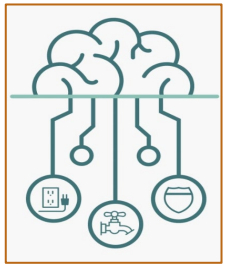
Data: On Field Sensors

Models: Edge & Near Edge



Data/Models: Cloud

Data/Models: HECs



ICICLE-enabled Computing Continuum

Potential for the ICICLE Solutions to be applied to more Verticals

Smart Foodsheds

Digital Agriculture

Animal Ecology

Health & Medicine

Environment

Communications & Collaboration

Mobility, Machines, & Manufacturing

AI for Social Good

ICICLE: Intelligent CyberInfrastructure with Computational Learning in the Environment

Systems AI Foundational Research for CI

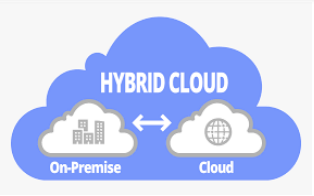
Intelligent Cyber Infrastructure

CI for AI

AI for "CI for AI"

On Field Sensors

Edge & Near Edge

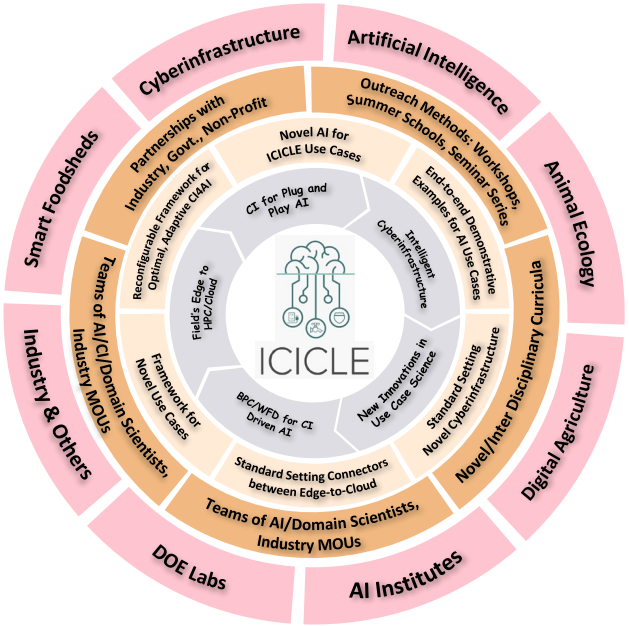


Clouds

HPC Systems & Data Centers

Emerging Computing Continuum

ICICLE Enabling Global Leadership in `Computing + AI'



Join Us!

- **Integrate into the National CI Ecosystem**
- **Integrative and Interoperable**
- **Leverages existing recognized capabilities**
  - Centers of Excellence, AI Institutes, Large Facilities
- **Collaborative**
  - Actively engaging CI experts, domain scientists,
  - AI/CI Users and developers
- **Sustainable and Inclusive**
  - Workforce Development, Broadening Participation, Collaboration and Knowledge Transfer
  - Benefits other institutes, large facilities, and all sciences beyond lifetime of award

Acknowledgments to all ICICLE Participants (Faculty, Students and Staffs)

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Thank You!