Challenges for AI in Computational Sustainability

Carla P. Gomes
Cornell University

CompSustNet

Accelerating Science: A Grand Challenge for AI

AAAI Fall Symposium

November 17-19, 2016

Arlington, VA, United States

Thank you!

Expeditions in Computing (CISE)

→1st Expeditions in Computational Sustainability (2008)

Conference, Referred CompSust Tracks, Workshops

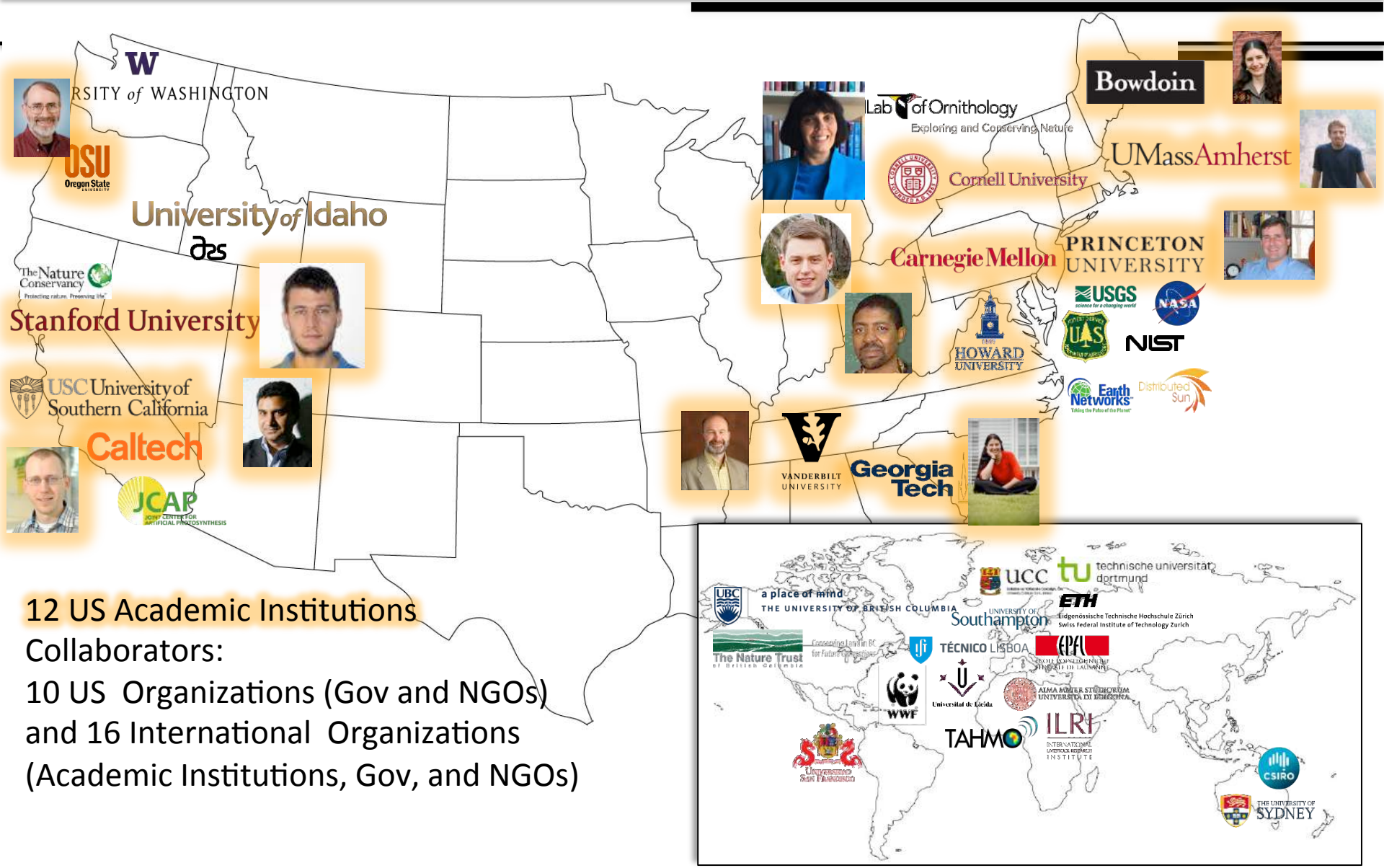
- **To nucleate** the Computational Sustainability field
- **To identify** a number of **core research directions** for **maximal impact**, both in terms of **Computer Science** and **Sustainability.**

→ 2nd Expeditions: Large-Scale Research Network (2015) for Expanding the Horizons of Computational Sustainability

CompSustNet

125+ faculty, students, and collaborators!!!

CompSustNet:
Large-scale Research Computational Sustainability Network



12 US Academic Institutions

Collaborators:

10 US Organizations (Gov and NGOs)

and 16 International Organizations

(Academic Institutions, Gov, and NGOs)

Computational Sustainability

Computational Sustainability: Advancing Computer Science and Sustainability Science

Computational Sustainability new interdisciplinary field that aims to advance computational methods to help balance economic, environmental, and societal needs for sustainable development.

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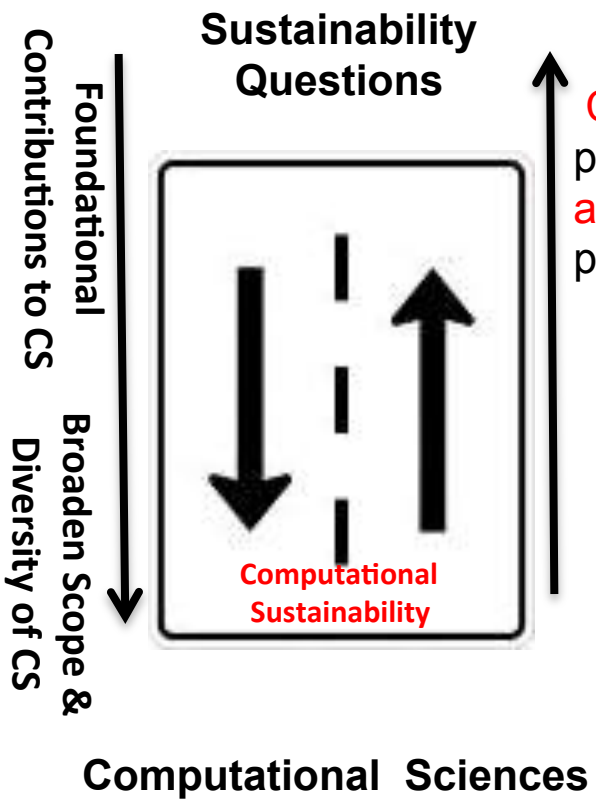
1. New challenging problems

2. New formalisms and concepts from other disciplines

→ **New Core Paradigmatic problems in Comp. Sci.**

→**Broadening the Scope & Diversity in CS**



Computational Thinking that will provide new insights, methodologies, and solutions to sustainability problems

→ **Societal Impact**

Challenges in Decision-Making for Managing Complex Natural and Man-Made Eco-Systems

Economic Model

e.g. combinatorial auctions

Complex Natural and Man-Made Ecosystem

Decision-Making (Management and Prediction)

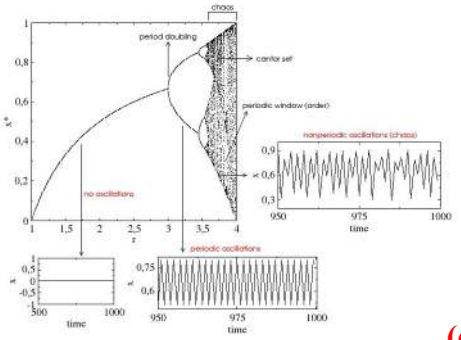
Wind, solar, water

Non-linear Dynamics

Plants and animals

Ev and grid batteries

Resources



Nonlinear Dynamics: Logistics map

(simple population model)

$x_{t+1} = r\, x_t\, (1 - x_t)$,

r is the growth rate

For certain values of r →

chaotic behavior

(difficult to make predictions even for deterministic models)

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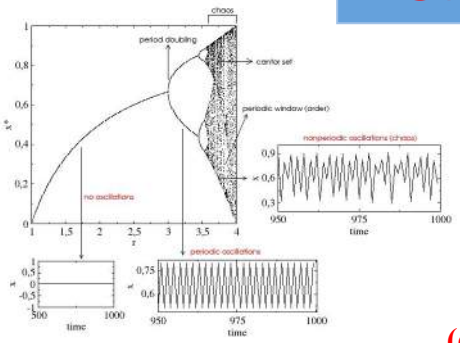
Non-linear Dynamics

Gaussian noise, heavy-tails, bursts, rare-events, lagged processes, temporal and model uncertainty, …

Uncertainty



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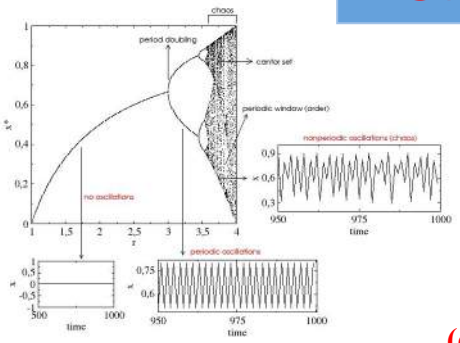
Non-linear Dynamics

Multiple temporal and spatial scales

Multiple climate scales
Multiple ecological scales
Multiple energy scales …

Gaussian noise, heavy-tails, bursts, rare-events, lagged processes, temporal and model uncertainty, …

Uncertainty



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Sustainable development
Multiple time scales
Meeting present needs (short-term) without compromising the needs of future generations(long-term)

Challenges in Decision-Making for Managing Complex Natural and Man-Made Eco-Systems

Economic Model

Complex Natural and Man-Made Ecosystem

Multiple Agents Often with Conflicting Preferences

Gaussian noise, heavy-tails, bursts, rare-events, lagged processes, temporal and model uncertainty, …

Decision-Making (Management and Prediction)

Wind, solar, water

Plants and animals

Ev and grid batteries

Resources

Non-linear Dynamics

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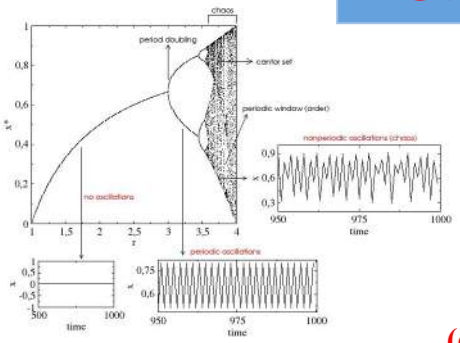

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Uncharted Territory for Computer Scientists
Optimization problems
(discrete and continuous variables) with
underlying complex dynamics under uncertainty
over multiple scales and multiple objectives

CompSustNet: 3 Core Sustainability Themes

Over 20 Novel Interdisciplinary Research Projects (IRPs)

I Conservation and Biodiversity

Bird Conservation
Prioritizing Conservation Decisions
Wildlife Corridors
Protecting Endangered Species

II Balancing Socio-economic Needs

Improving Weather Observations in Africa
Protecting Migratory Herders in Africa
Social-economic ecological corridor (Ecuador)
Poverty Mapping

III Renewable Energy, Accelerating Discovery of Sustainable materials, and Smart Cities

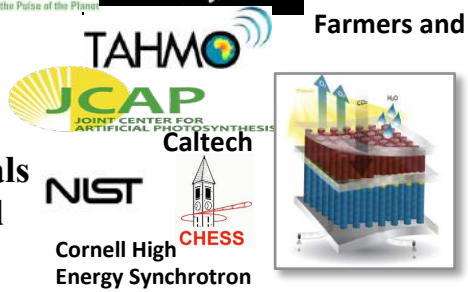
Accelerating the Discovery of New Sustainable Energy Materials
Energy Storage and Integration of Renewables In Smart Grid
Smart Bike Sharing

Bird Conservation

Wildlife Corridors
Social-economic
ecological corridor
(Ecuador)

Elephant Listening Proje
Green Security Games

Farmers and Migratory Herders in Africa



Cornell High
Energy Synchrotron

Solar Fuels

Smart Bike Sharing

Smart Grid

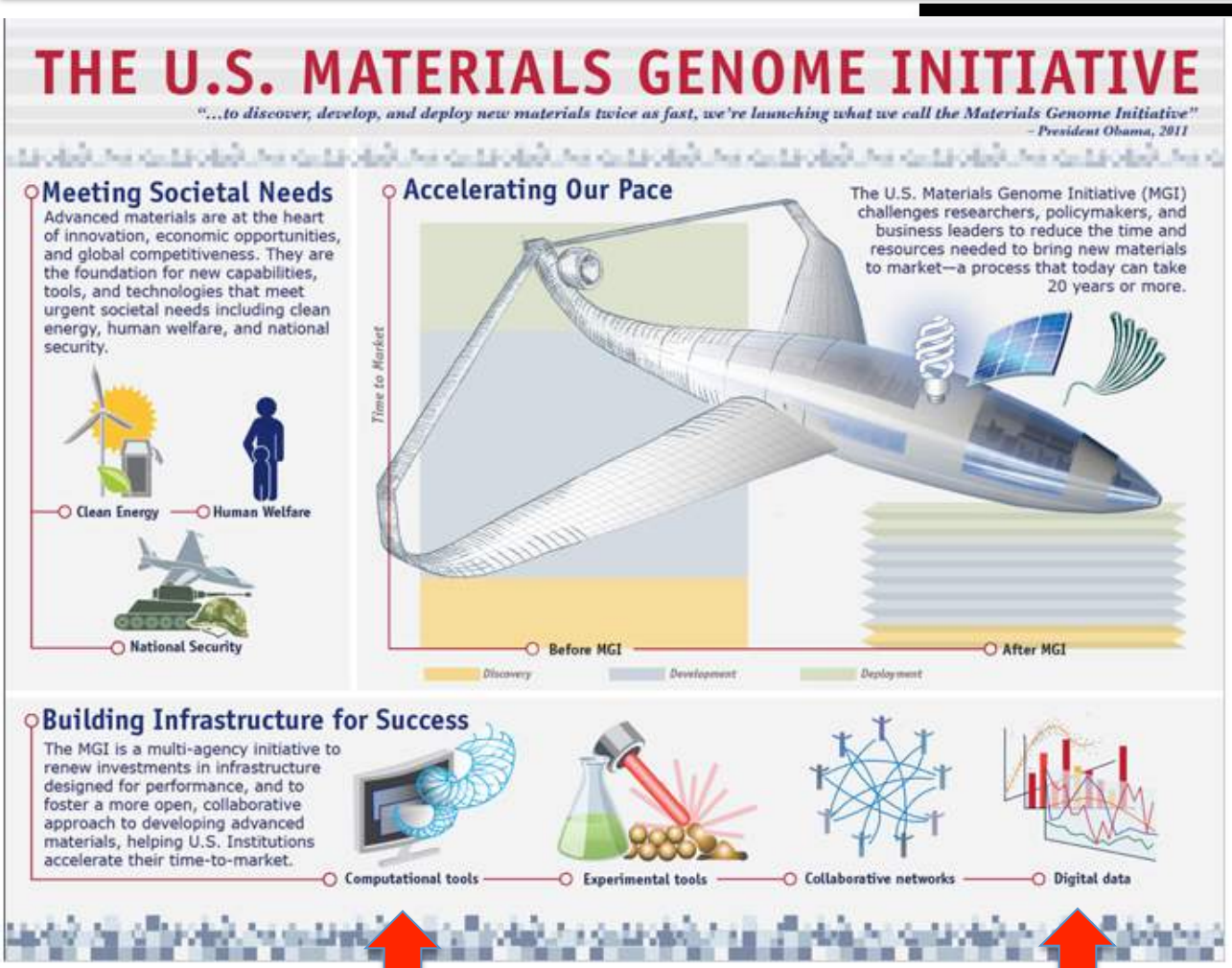
Wide range of sustainability applications:
To build a ***coherent and cohesive computer science sub-field*** it's paramount to **go deep** in terms of **Cross-Cutting Core Computational Problems** and apply them to different sustainability areas.

Accelerating
Materials Discovery for Sustainable Energy

Artificial Tree

(solar-fuel generator)

White House Materials Genome Initiative



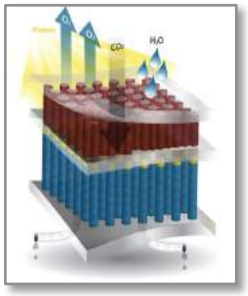
Goal:

Accelerate the pace and reduce the cost of discovery and deployment of advanced material systems

Very exciting new research area for Computer Science with tremendous potential for impact

Accelerating the Development of Solar Fuel Generators

"… existing energy approaches […] *will not be enough to secure our energy future. Meeting the challenge will require […] scientific breakthroughs in new materials….*"
Report of Dept. of Energy [2010]



Solar fuel Cell

Artificial Tree
(solar-fuel generator)

Solar fuels can be substantially produced and stored

Our goal
accelerate the development of solar fuel generators

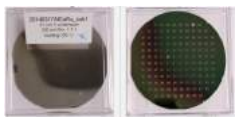
JCAP Caltech
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

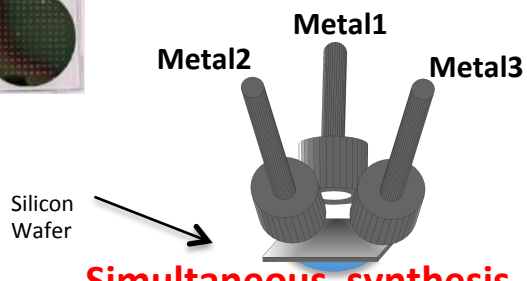
SLAC
Stanford Linear Accelerator

CHESS
Cornell High-Energy Synchrotron

Discovering better catalysts for solar fuel generators

Co-sputtering
(similar to atomic spray painting)

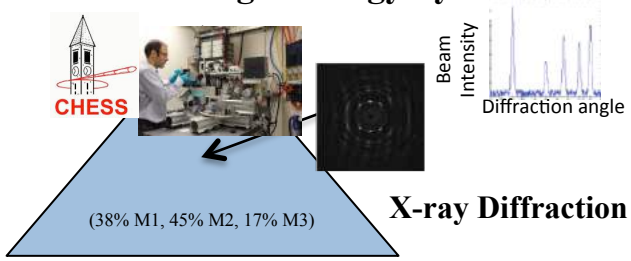




Simultaneous synthesis
of thousands of materials

High-Throughput
Materials Discovery

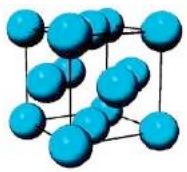
Cornell High-Energy Synchrotron



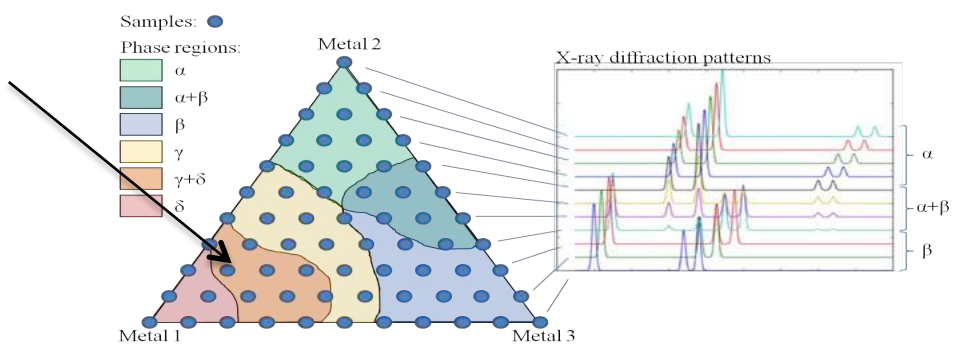
X-ray Diffraction

Rapid characterization
of thousands of materials

How to determine the crystal structure
of the materials, based on the X-ray diffraction patterns?



FCC Crystal Structure



Goal:
Achieve High-Throughput Crystal Structure Identification

Crystal Structure Map
Problem:
Infer the crystal structures of the materials from the X-ray diffraction patterns

(currently a largely manual process, requiring expert knowledge)

Source Separation Problem

Difficulty: Often X-ray diffraction patterns correspond to a mixture of crystal structures

Challenging to un-mix the X-ray diffraction patterns

JCAP JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS
Caltech

Crystal Structure Map Problem

$$0 \le I_{p,k} \le 1 \; k = 0, \cdots, K-1, p = 0, \cdots, P-1$$

$$r_{p,k} \Leftrightarrow (I_{p,k} = 1) \; k = 0, \cdots, K-1, p = 0, \cdots, P-1$$

$$\bigwedge_{k=1}^{K-1} (r_{0,k} \Rightarrow r_{0,k-1})$$

$$\cdots$$

$$\bigwedge_{j=1}^{K-1} \left(\left(\bigwedge_{i=0}^{Y} \neg r_{i,j} \right) \Rightarrow \bigwedge_{k=j}^{K-1} (r_{Y+1,k} \Rightarrow r_{Y+1,k-1}) \right)$$

$$\bigvee_{k=0}^{K-1} \bigvee_{\ell=0}^{L-1} (r_{p,k} \wedge (|e_{k,\ell} + S_{p,k} - a| \le \epsilon)) \forall p, \forall a \in \mathcal{A}(p)$$

$$\left(\bigwedge_{i=0}^{t-1} (S_{d_i,k} \ge S_{d_{i+1},k}) \right) \vee \left(\bigwedge_{i=0}^{t-1} (S_{d_i,k} \le S_{d_{i+1},k}) \right), k = 0, \cdots, K-1$$

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$$\left(\left(\sum_{k=0}^{K-1} I_{p,k} = 3 \right) \wedge \bigwedge_{k=0}^{K-1} (r_{p,k} \Leftrightarrow r_{p',k}) \right) \Rightarrow (S_{p,k} = S_{p',k}), \forall p, \forall p' \in \mathcal{N}(p)$$

Sat Modulo Theory Formal Specification of Crystal Structure Map Problem

Standard techniques
fail to capture the underlying physics of the phenomena

Rich set of combinatorial constraints
to capture the physics and
the relationships among
thousands of
X-ray diffraction patterns.

Computational Synthesis:

Integration of machine learning techniques with constraint and probabilistic reasoning, sampling, and optimization techniques

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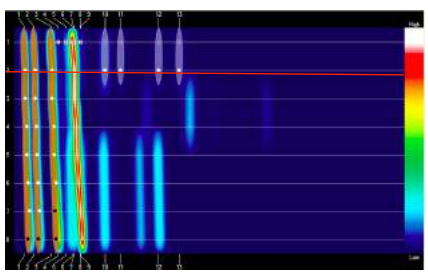


Heatmap of X-Ray patterns

UDiscover.It

Puzzles, Games, Tasks

Cornell Summer College
EXPLORATIONS IN ENGINEERING
ENGRG 1060
~ 90 High-School students

Amazon Mechanical Turk

Human Computation - Crowdsourcing,
minimal visual pattern information,
based on
the heatmaps of the X-ray diffraction patterns,
can lead to further speed ups
(from hours to minutes)

Beautiful but challenging research problem for CS!
Solving it will accelerate dramatically
the discovery of new materials for solar fuels!

High-Throughput Crystal Structure Discovery

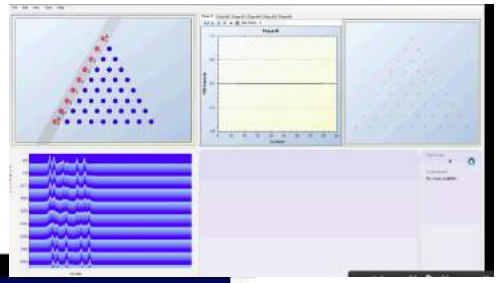
Theory

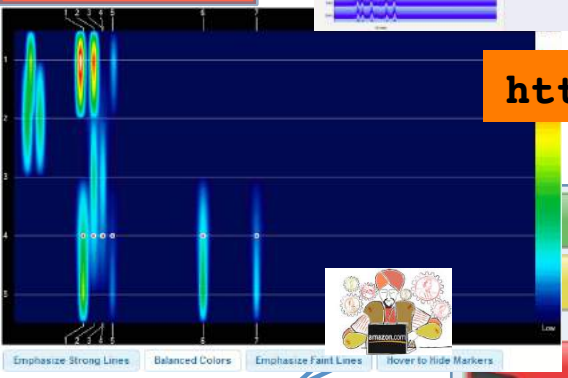
High-throughput Synthesis

Scientific Literature & Databases

Human Computation Expert and Non-Expert

Human Input: Intermediate Level





Human Input
General Public, K-12

Crowdsourcing

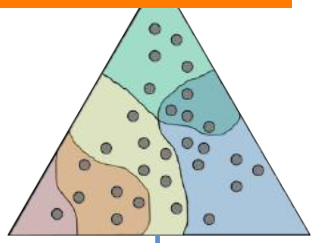
Theory

Scientific Literature & Databases

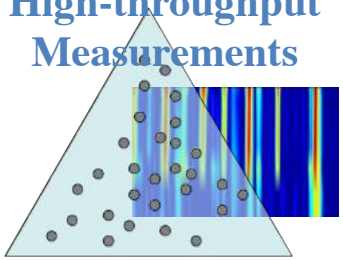
Planning and Design of Experiments: Robotics Lab

Active Learning

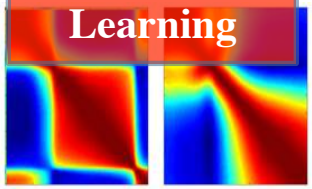
http://www.udiscover.it



High-throughput Measurements



Data Mining and Machine Learning



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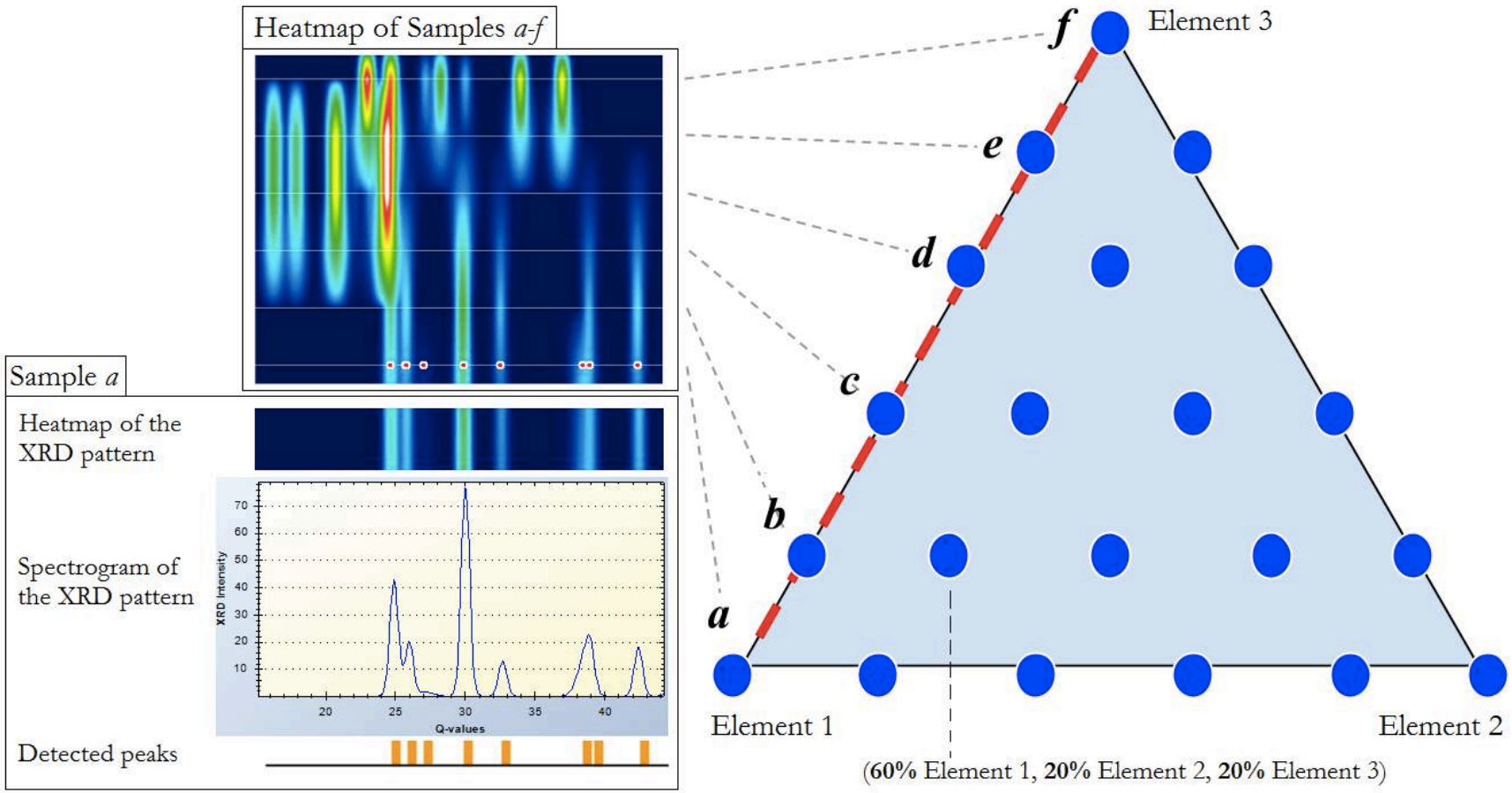
Probabilistic, Constraint Reasoning & Optimization, Matrix Factorization

Underlying Physics
(e.g., XRD Shifts, known phases, lattice structure and lattice parameters, etc)

Decomposition:
Slices of Sample Points
Different Visualizations of X-Ray Diffraction Patterns

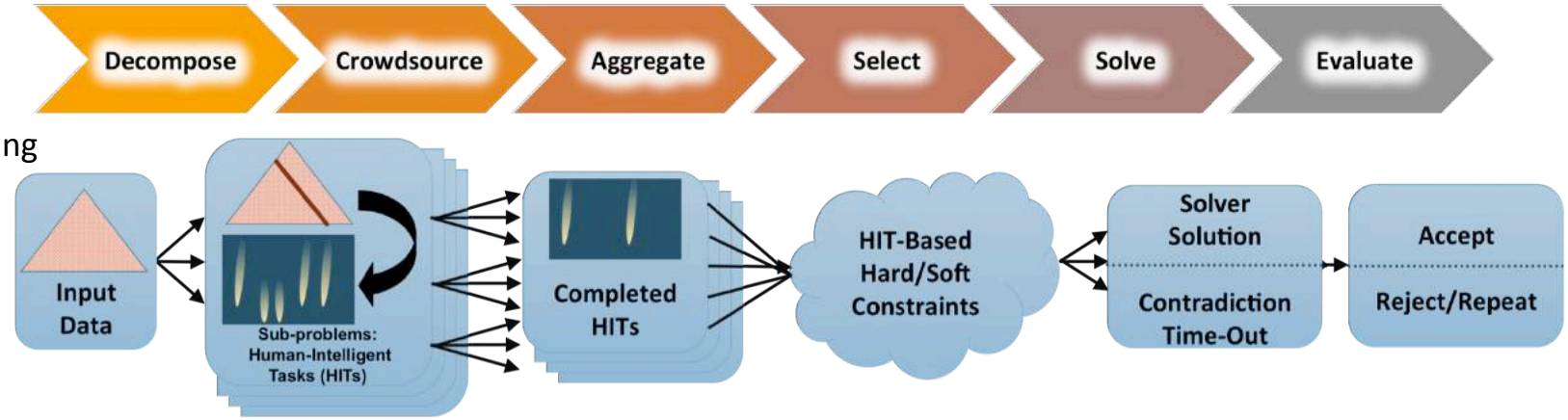


Human Computation Framework for Boosting Combinatorial Solvers

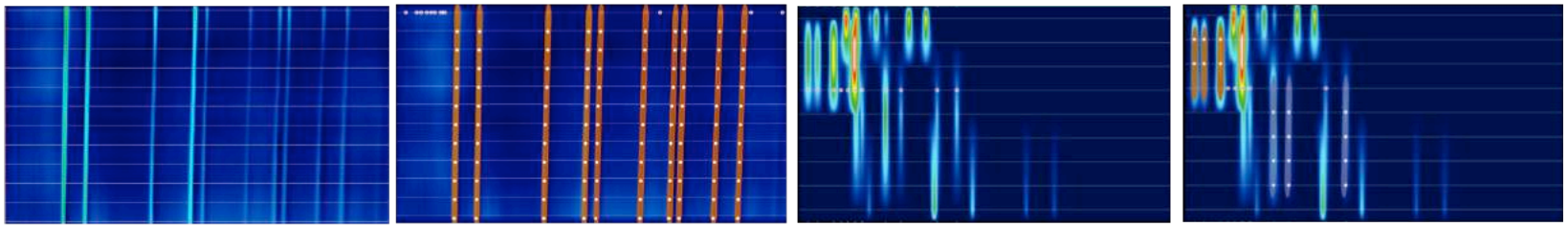
www.Udiscover.It

Top: Human-Machine Framework

Edge matching puzzle



Bottom: Human Intelligent Tasks (Hits)



1.a) 1.b) 2.b) 2.b)

Ronan Le Bras, Yexiang Xue, Richard Bernstein, Carla P. Gomes, Bart Selman, HComp14

www.Udiscover.It

U-DiscoverIt: CrowdSource Mechanical Turk

System	Dataset P	L^*	K	#var	#cst	Time w/o user input (s)	Time w/ user input (s)	# assigned var. by user
A/B/C	36	8	4	408	2095	3502	859	19 (4.6%)
A/B/C	60	8	4	624	3369	17345	4377	18 (2.9%)
Al/Li/Fe	15	6	6	267	1009	79	4	6 (2.2%)
Al/Li/Fe	28	6	6	436	1864	346	62	12 (2.7%)
Al/Li/Fe	28	8	6	490	2131	100[illegible]	[illegible]	[illegible]
Al/Li/Fe	28	10	6	526	2309	281	[illegible]	[illegible]
Al/Li/Fe	45	7	6	693	3281	188	[illegible]	[illegible]
Al/Li/Fe	45	8	6	711	3410	46816	1003	30 (4.2%)

Human Computation:
From ~13 hours to 1000 seconds!

Table 1: Runtime of SMT solver with and without user input. P is the number of sample points, L^* the average number of peaks per phase, K the number of basis patterns, #var the number of variables and #cst the number of constraints.

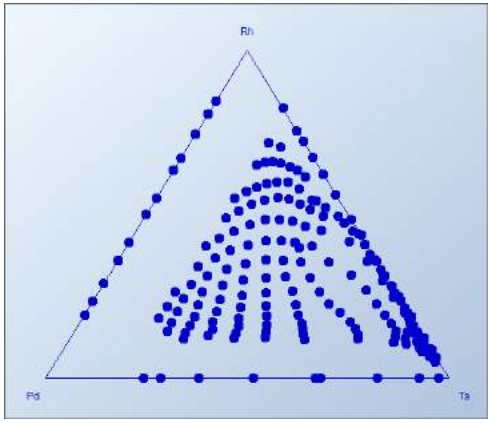
Human input can dramatically speed up the performance of combinatorial optimization methods (identification of backdoor variables).

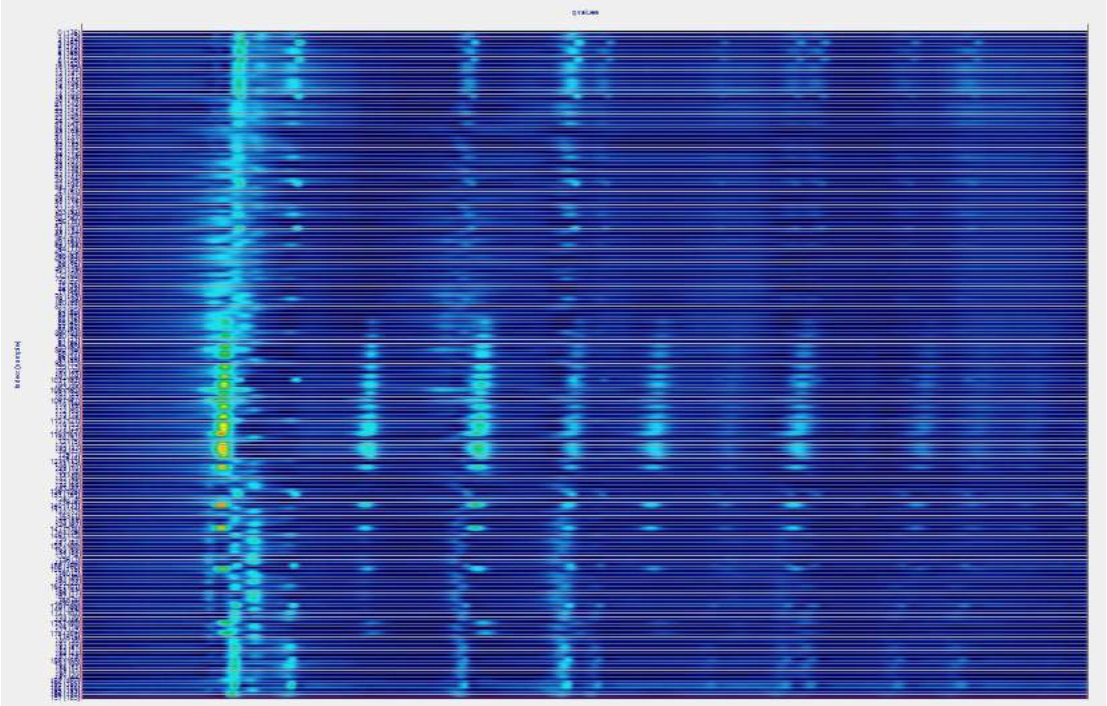
Approaches leverages the complementary strength of human input, providing global insights into problem structure, and the power of combinatorial solvers to exploit complex constraints.

Le Bras, Bernstein, Gomes, Selman and van Dover 2013

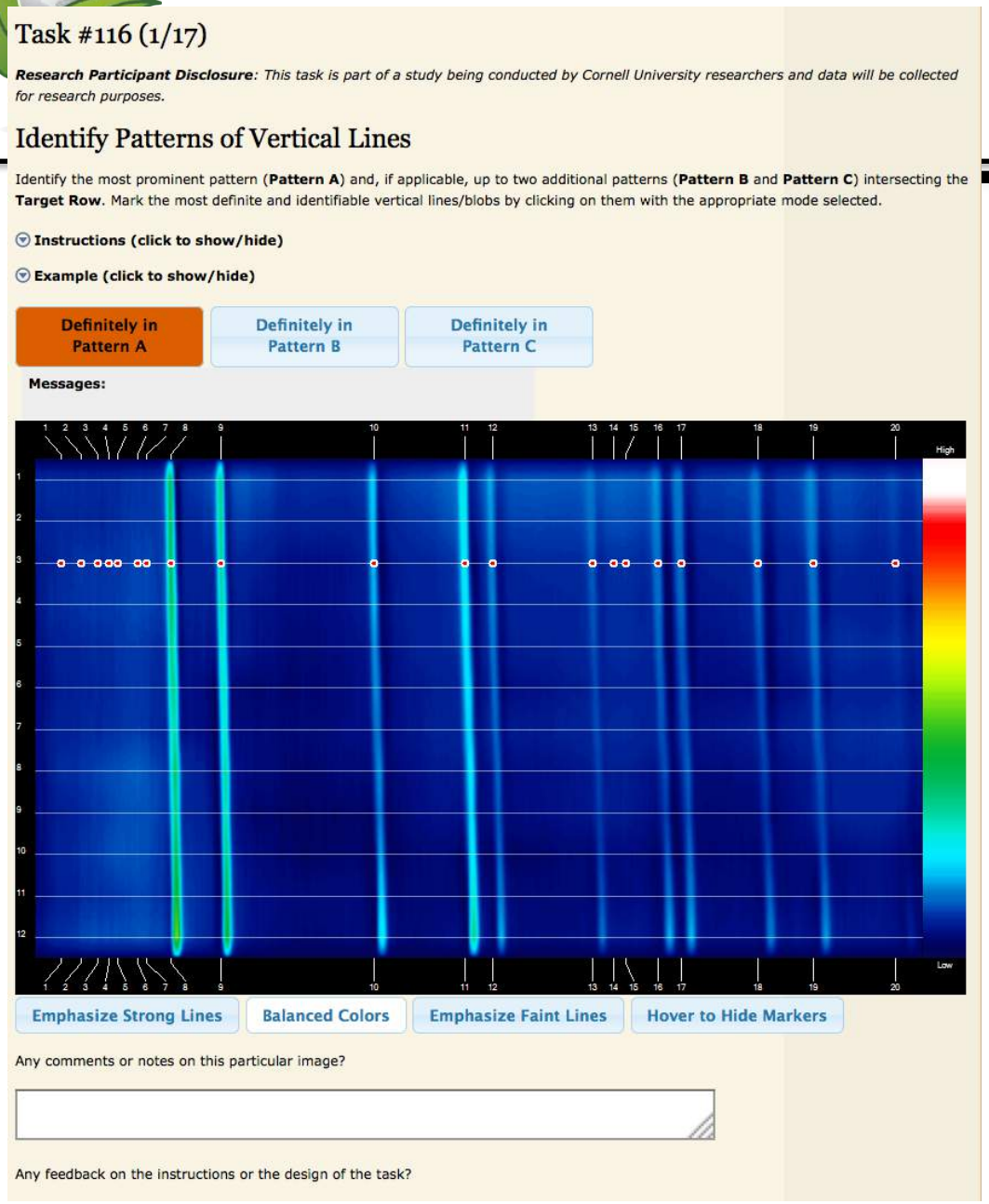
Real System: Pd-Ta-Rh system

198 synchrotron
x-ray diffraction patterns





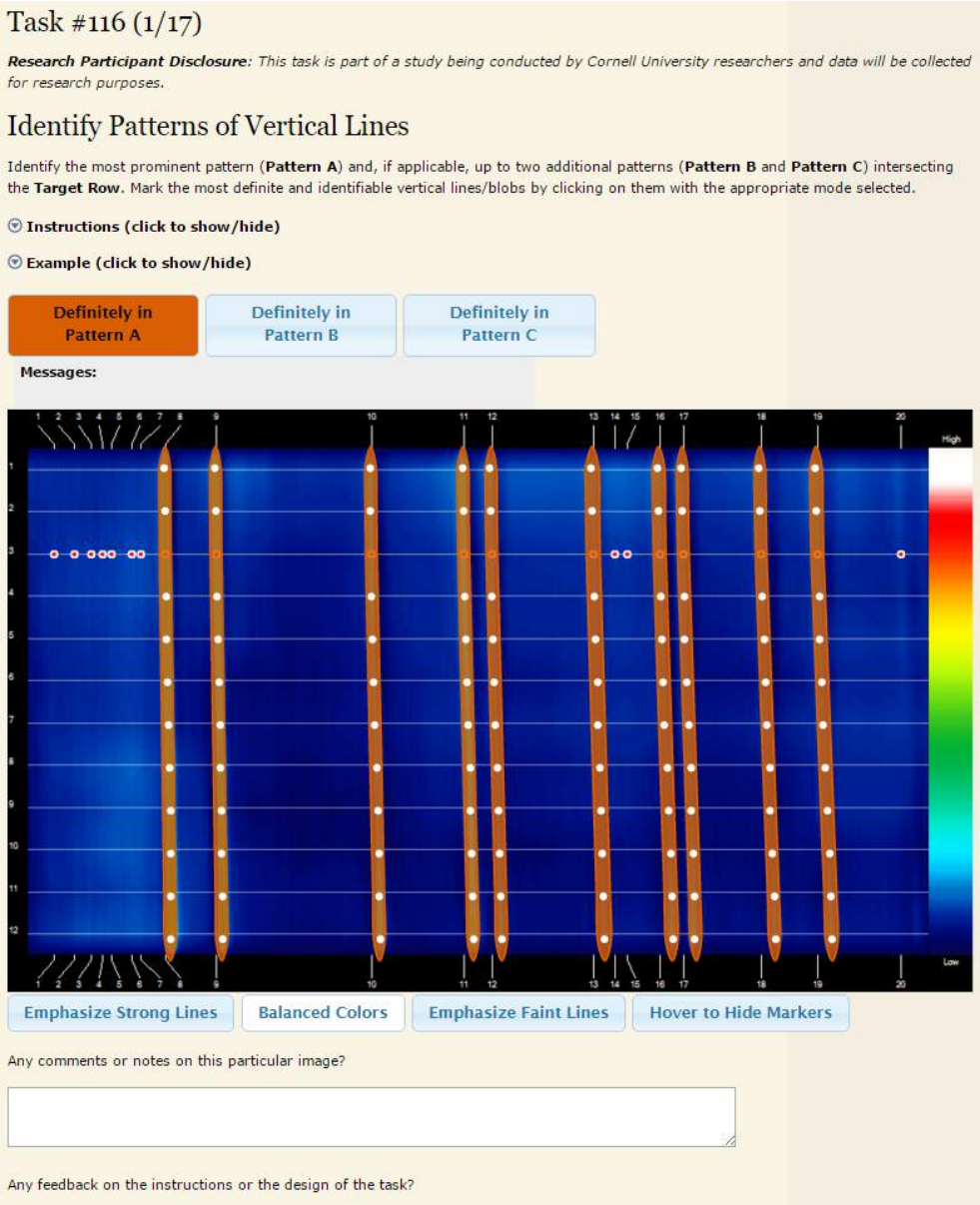
UDiscoverIt: Task #116



Cornell Summer College
EXPLORATIONS IN ENGINEERING
ENGRG 1060
~ 90 students
(Bruce van Dover)

Amazon Mechanical Turk

UDiscoverIt



84 % participants answered that this slice involves 8 or more peaks

Cornell Summer College
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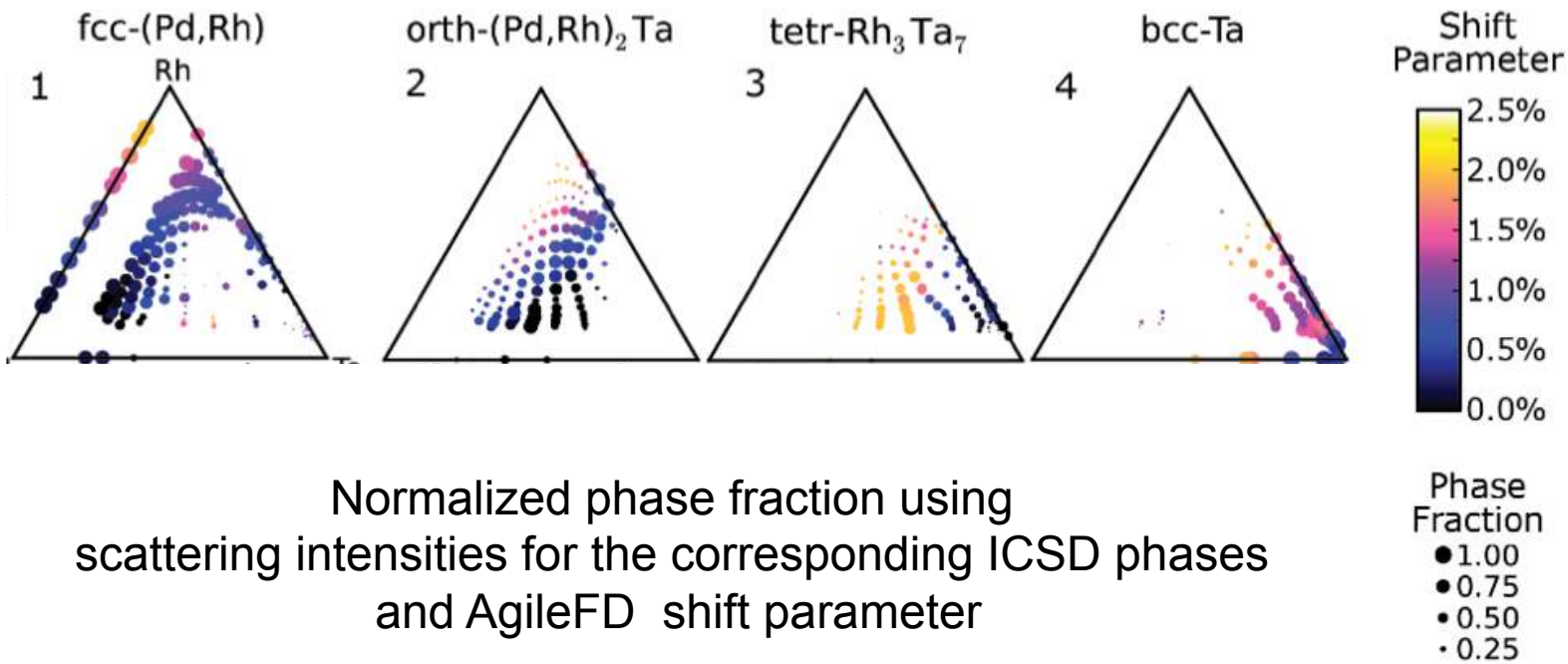
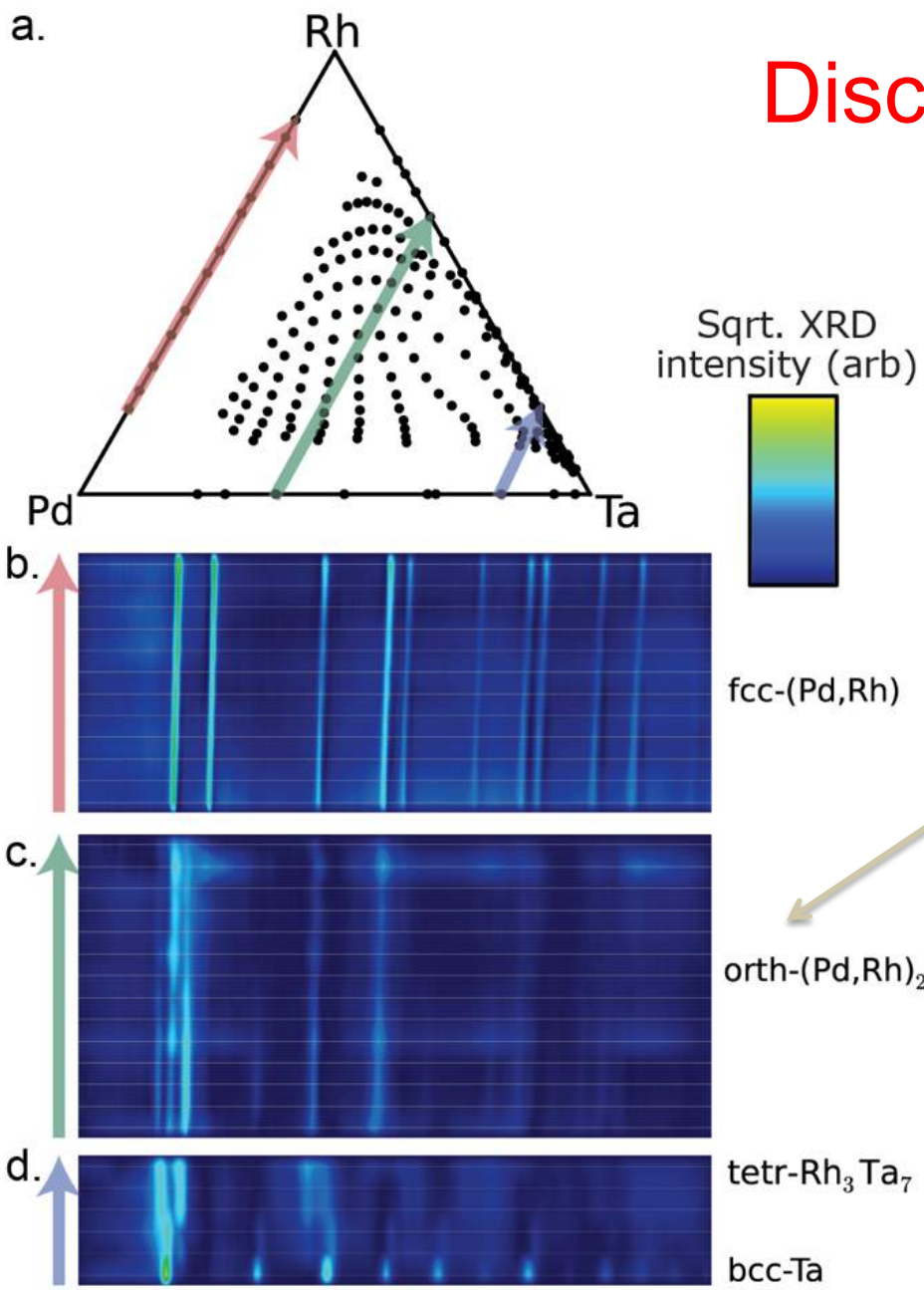
Incorporating Insights form the Crowd into AgileFD, a Convolutional Matrix Factorization Algorithm

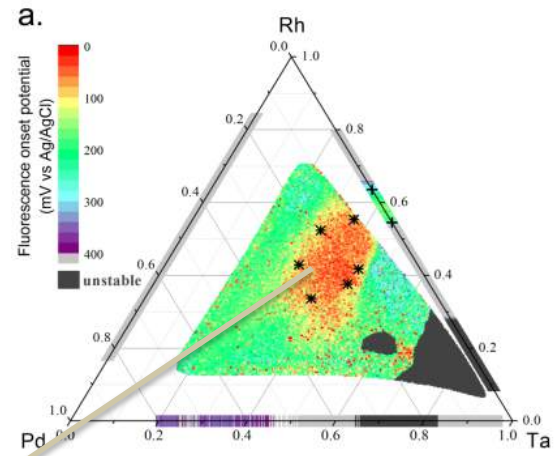
Our approach with Human Input



Normalized phase fraction using scattering intensities for the corresponding ICSD phases and AgileFD shift parameter

Pd-Rh-Ta System: Discovery of a New Material



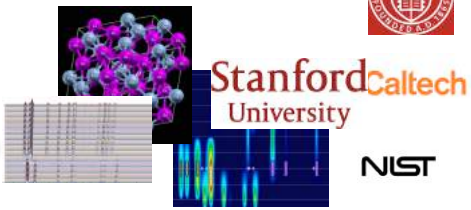


orth-(Pd,Rh)$_2$Ta

$Pd_{0.14}Rh_{0.40}Ta_{0.46}$ → best known Pt-free catalyst for methanol oxidation

CompSustNet's
Cross-Cutting Computational Themes

Cross-Cutting Computational Theme:
Pattern Decomposition in Big Data



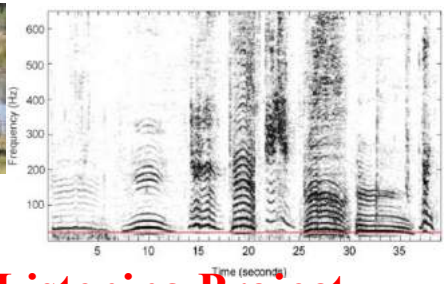
Stanford University Caltech NIST JCAP CHESS Caltech

High Throughput Materials Structure Identification

Dimensionality reduction with complex constraints

Caltech Carnegie Mellon University Stanford University

Similar computational problems:
Both involve the decomposition of a signal (X-rays / audio) into patterns (crystal structures / types of sounds)



University of Southampton

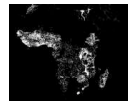
Elephant Listening Project

Project to monitor elephant populations by analyzing forest recordings

Our Philosophy:
Students should work on similar computational problems in different domains.
Grad students working on materials discovery also work on the elephant calls.

We represent these cross-cutting computational themes with colored "subway lines."
Pattern Decomposition in Big Data is the blue line.

Subway Lines: Examples of Cross-Cutting Computational themes and Interactions of some of CompSustNet's projects



Poverty Mapping and Targeting

Bike Sharing

Dynamic Precision Bird Conservation

Large-scale Socio-Economic Modeling of Pastoralists' Movements (Kenya)

National Wildlife Refuge System

- Pattern Decomposition in Big Data
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- Agents: Mechanism Design
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Landscape-Scale Conservation and Rural Communities (Ecuador)

eBird

Citizen Science **Avicaching** , Estimating Bird Populations and Migrations

Wind & Solar Forecasting

Design and Control of Electricity Storage Systems

Monitoring Sea Star Wasting Disease Outbreak

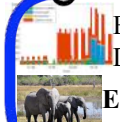
Characterization of Power Grid State

eButterfly

New Forest Cicada Detection

adapt-N

Nitrogen Management



Electricity Usage Disaggregation

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High Throughput Materials Structure Identification

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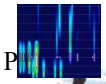
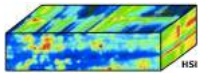
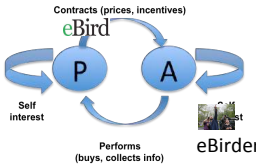




GrazeIt



TAHMO

Low-Cost Weather Stations in Africa (TAHMO)

www.Udiscover.It

Sustainability Themes:

Biodiversity and Conservation

Balancing Socio-Economic Needs

Computational Themes:

Small Data / Big Data:

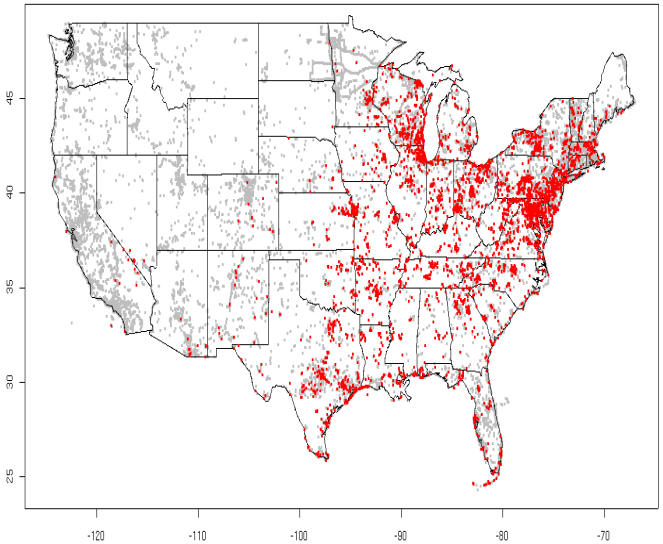
Citizen Science, Learning, Mechanism Design and Dynamical Stochastic Optimization

Citizen Science plays a key role in Bird Conservation

300K+ volunteer birders	300M+ bird observations	22M+ **hours of field work** (2500+years)

eBird

CORNELL LAB of ORNITHOLOGY

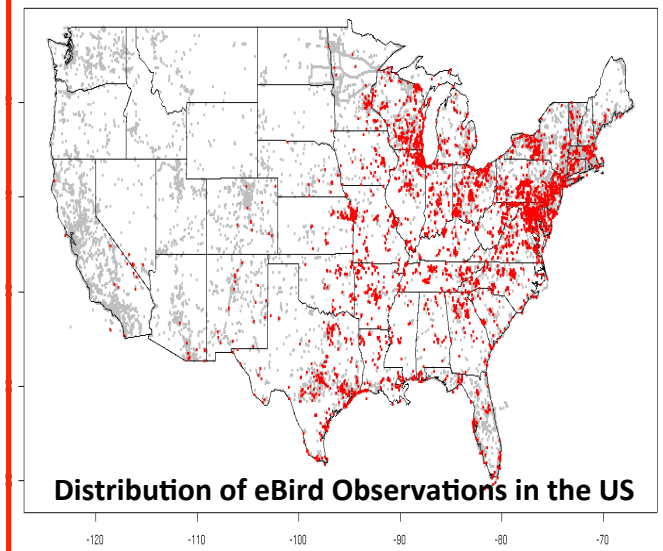


Distribution of eBird Observations in the US

Challenge:
Biased data,
mainly from urban areas

Avicaching:
A Two Stage Game for Incentivizing Bias Reduction in Citizen Science

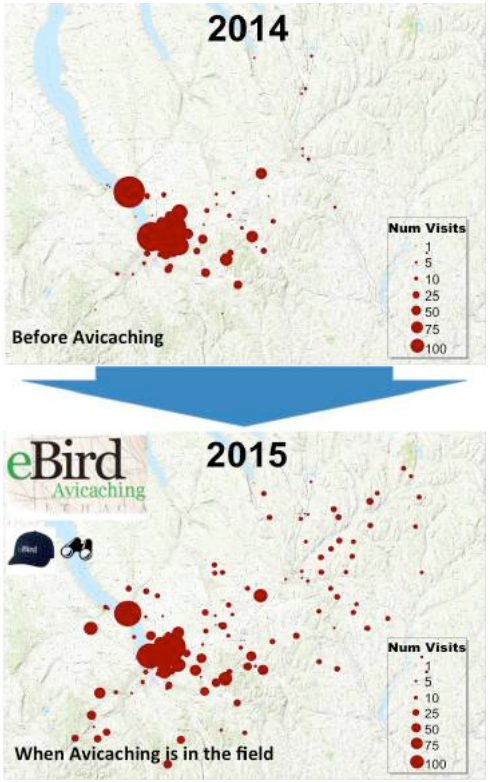
Data Bias Problem



Prevalent problem in citizen science
Collected data are often aligned with the participants' preferences rather than scientific objectives.

How to incentivize Citizens to visit under-sampled areas?

Principal-Agent Framework



Very Successful in Two US Counties (19% shift to undersampled areas in a 6 month period)

Field: Pilot Program

Incentivize eBirders to visit undersampled locations.

Incentives:

- Avicaching points,
- leaderboards
- Lotteries (e.g. binoculars.)

Yexiang Xue, Ian Davies, Daniel Fink, Christopher Wood, Carla P. Gomes, AAMAS 2015, CP 2016, NIPS 2016

Bird Distributions

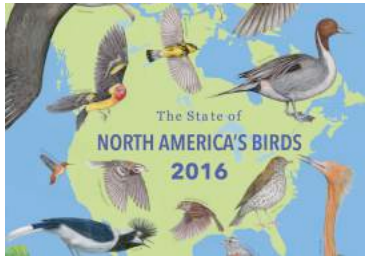
Machine Learning and Citizen Science

eBird

Bird Observations

300K+ volunteer birders	300M+ bird observations	22M+ **hours of field work** (2500+years)

State of the Birds Report
(officially released by Secretary of Interior)



Novel Approaches
To Conservation
Based on eBird Models

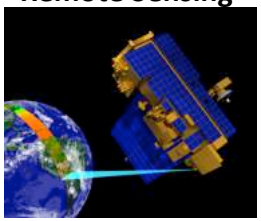
Distribution Models for 400+ species with weekly estimates at fine spatial resolution ($3km^2$)

Environmental Data

Land Cover

Weather

Remote Sensing

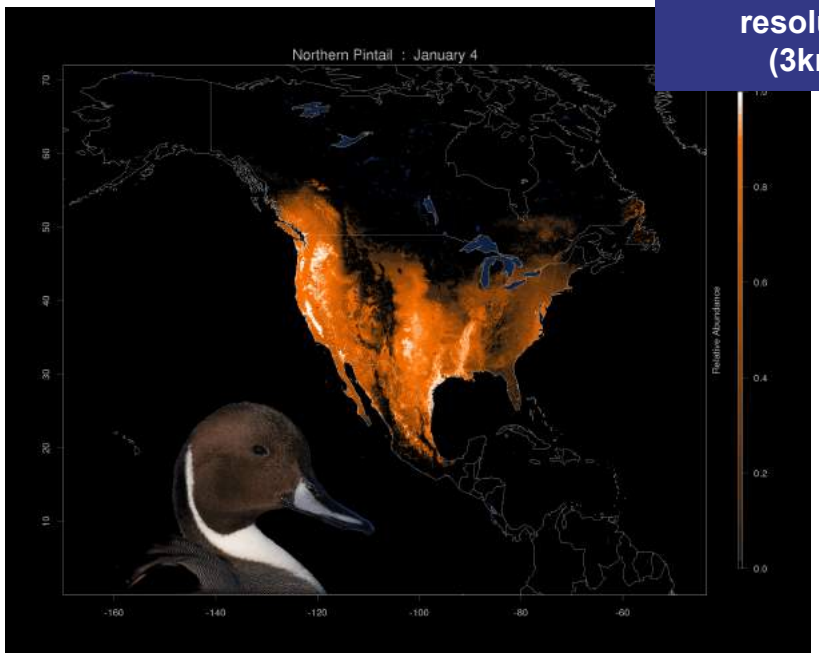


TeraGrid

80,000+ CPU Hours (~ 10 Years!!!)

Adaptive Spatio-Temporal Machine Learning Models and Algorithms (STEM Models)

Relate environmental predictors to observed patterns of occurrences and absences



Patterns of occurrence of the Northern Pintail for different months of the year Source : Daniel Fink

Bird Distribution Models, Revealing, at a fine resolution, Species' Habitat Preferences

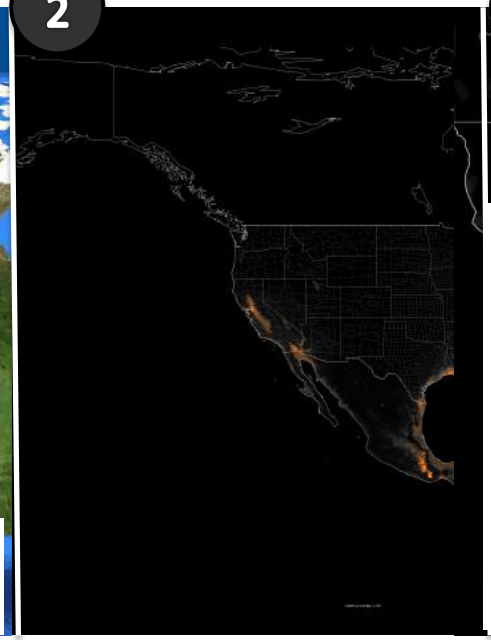
Dynamic High-Precision Conservation
Bird Returns

Protecting Migratory WaterBirds in California Against Drought

1

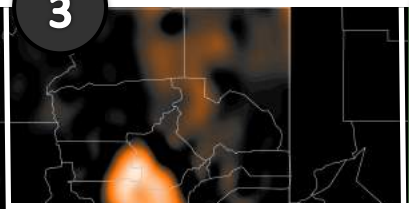
Pacific Migration Flyway

2



eBird Models

3



Target Estimates

4

Farmers Submit Bids

Reverse Auction Bid Selection

Using big data, machine learning techniques, and a market-based approach
The Nature Conservancy has generated
over 20,000 acres of additional habitat for waterbirds in California

Combinatorial Reverse Auctions

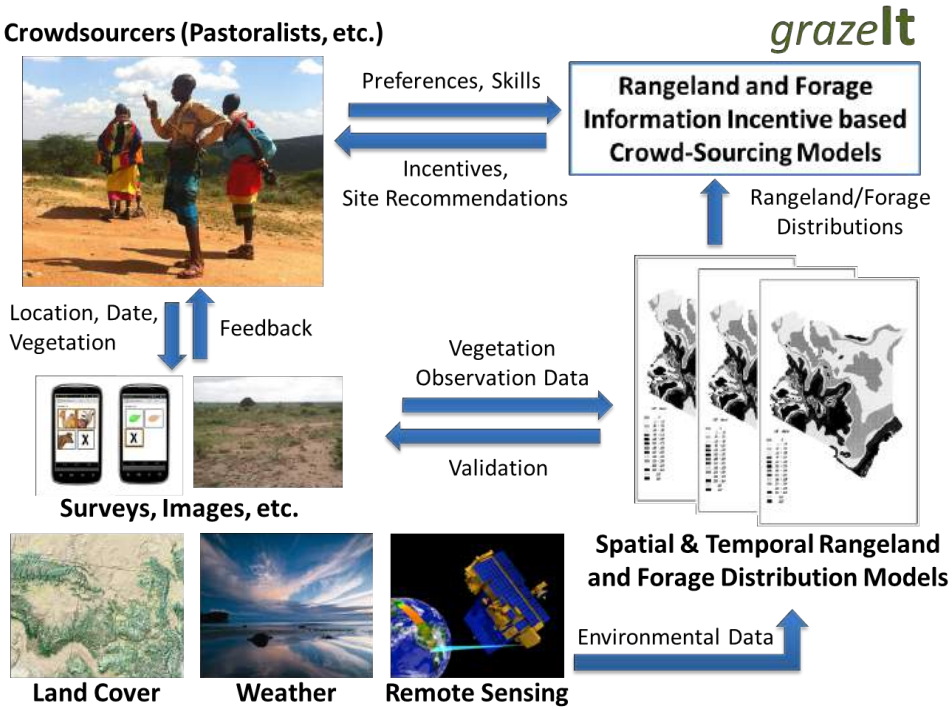
Sacramento Valley, CA

Farmers submit bids to TNC to keep the rice fields flooded during short periods of bird migration in California.

Radically novel, dynamic, way of doing bird conservation.
Only possible because of advanced computational methods.

Poverty Mitigation in Africa:
Big Data for Africa

Improving Weather, Rangeland, and Forage Maps in Africa
to protect farmers and herders



grazeIt

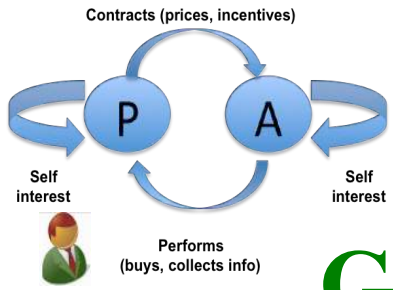
Herders Submit Vegetation Images and Surveys with Smartphones: incentives: real money (small for us, good money for pastoralists)

3 month Pilot project:
→ 100,000+ surveys

Africa is very poorly sensed
(limited environmental data, vegetation maps, only a few reliable weather stations)

Cross-Cutting Computational Theme

Findings can be transferred across domains!

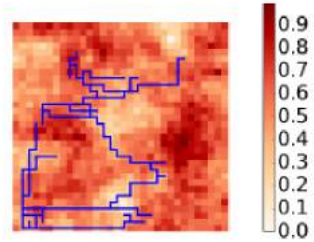


eBird Avicaching

GrazeIt

Mechanism Design: Principal-Agent Game-Theory Model

Landscape Connectivity for Andean Bears (Ecuador)



Where to place patrols to prevent poaching and illegal fishi

How to incentivize Citizens to visit under-sampled areas?

Computationally, these problems have similarities.

USC University of Southern California

Milind Tambe
Fei Fang

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Mechanism design is the baby blue line.

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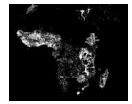

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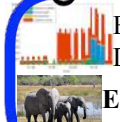

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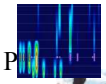

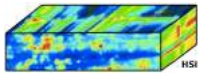

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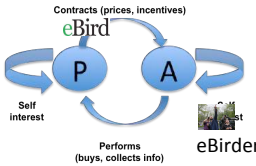

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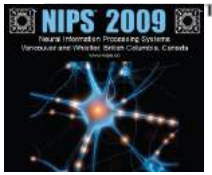
CoompSust@AAAI-2017

Vibrant Research Community

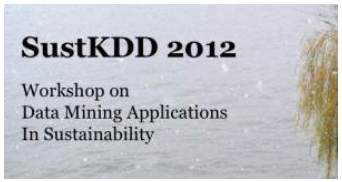
CompSust Conference Series:

(international researchers from several disciplines and institutions (universities, labs, government)

Workshops at Conferences



Neural Information Processing Systems Foundation



STOC 2012 – 44th ACM SYMPOSIUM ON THEORY OF COMPUTING

Tracks at Established Conferences

CROCS: Constraint Reasoning and Optimization for Computational Sustainability

CROCS at **CP**-09, **CPAIOR**-10 **CP**-10 and **CP**-12

Theme of IJCAI-2013 (CHINA) AI and Computational Sustainability

IJCAI-13

s

CompSust Virtual Seminar

www.compsust.net

And many other related conferences and journals

CompSustNet:
Large scale research network for Expanding the Horizons of Computational Sustainability

CompSustNet

Expeditions in Computing (CISE)

THANK YOU ☺!

125+ faculty, students, and collaborators!!!