

**DOE Bioenergy Technologies Office (BETO)
2021 Project Peer Review**

**Agent-based Modeling for the Multi-objective
Optimization of Energy Production Pathways:
Integrated Techno-economics and Life Cycle
Assessment**

March 12, 2021
Data Modeling and Analysis

Jason Quinn
Colorado State University



Colorado State University

B&D LLC

NC STATE UNIVERSITY

Project Overview

- *First of a Kind analysis project with bold goals*
- *Project goals: Develop open-source integrated US biofuel model that enables an evaluation from a systems level the ability to meet DOE sustainability goals*

What we are doing:

- Support informed research and commercialization direction based on economic and environmental goals
- Developing an integrated modeling framework

Why this is important:

- Sustainable US energy policy
- Biofuels portion of this picture
- Quantitative or measurable % reduction GHG, Cost, etc. of technology

How it is done today:

- Evaluate one technology scenario independent of other technologies
- Technology investment and policy are not typically fully informed

What are the risks:

- Large Scope
- Moving target

1 – Management

CSU Team



PI: Jason
Quinn



Co-PI: John
Field



Co-PI: Steve
Simske



Co-PI: Thomas
Bradley



RS I: Evan
Sproul



GRA: Jack
Smith

B&D LLC



Co-PI: Colin
Beal



TL: Nathan
Putnam



Co-PI: Jordan
Kern



GRA: Ece Ari
Akdemir



UG: Taylor
Pack

NCSU Team

Advisory Board



Troy Hawkins:
ANL



Carlos Quiroz-
Arita: SNL



Bill Brandt:
ASU



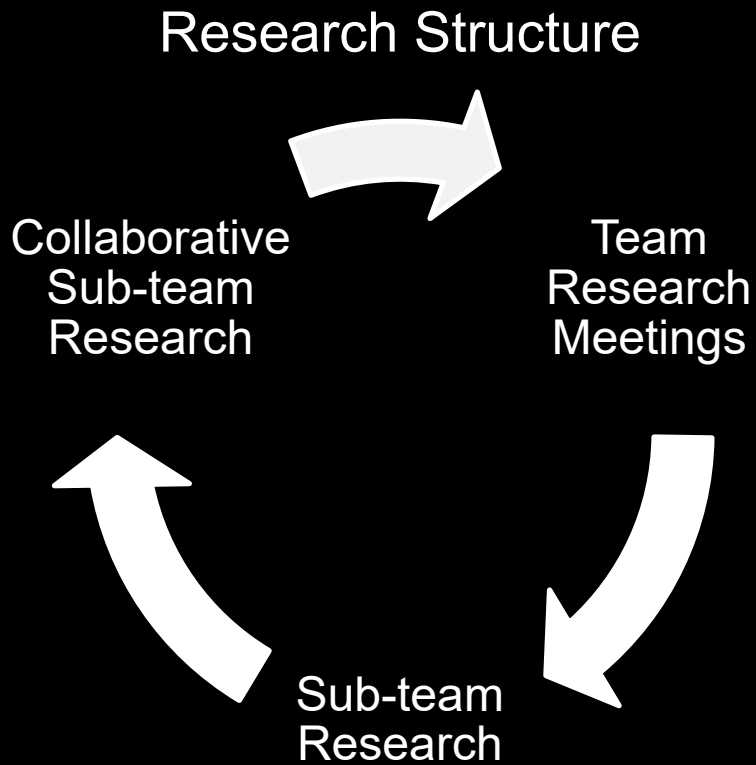
Ryan Davis:
NREL

1 – Management

Inclusive Research Environment

The Meeting Details:

- Weekly project meetings
- Quarterly meetings with DOE
- 6 month updates to Advisory board

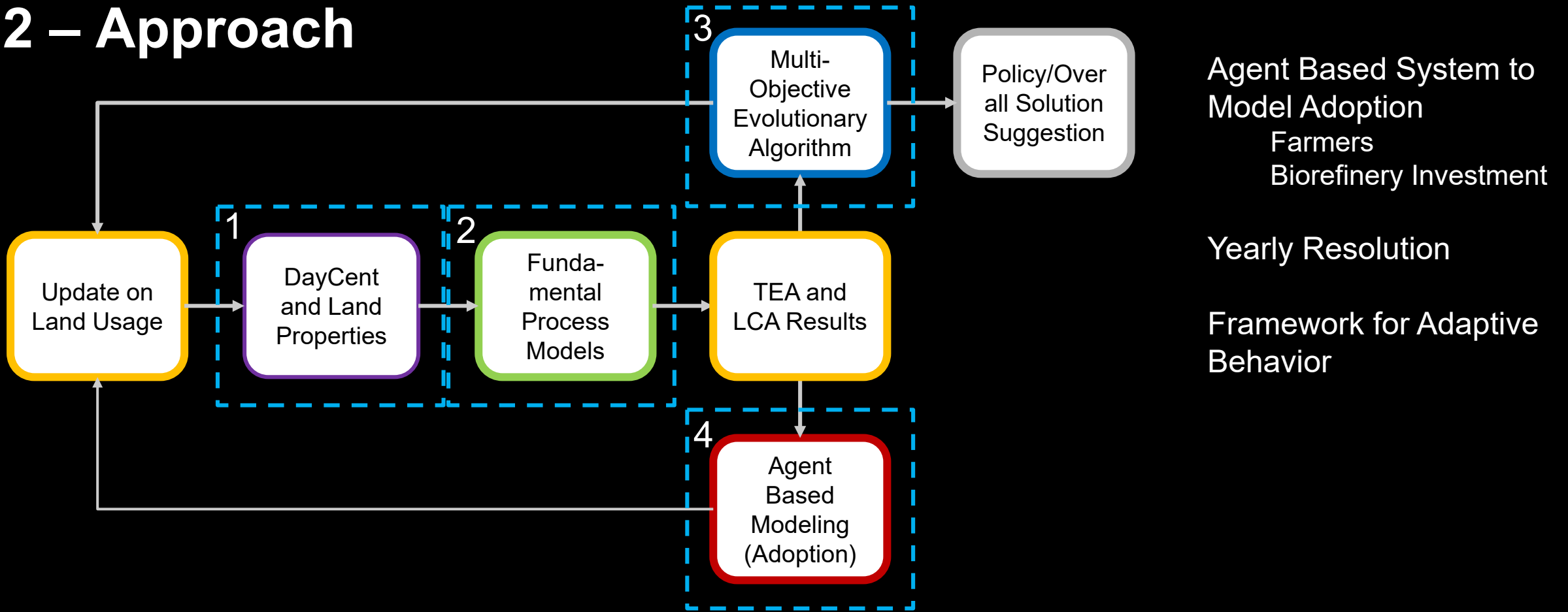


Risk Management:

Communication

Creative Problem Solving

2 – Approach



FOA targets:

- Reducing Consumption Water (10-30%), Energy Consumption (20-60%), GHG Emissions (50-80%), Pollutant Emissions (10-30%)

Program Connections:

- Optimization of the energy bioeconomy
- Defining from a systems level pathways and investments that lead to sustainable bio-economy

2 – Approach

DayCent: Geospatial Agricultural Modeling

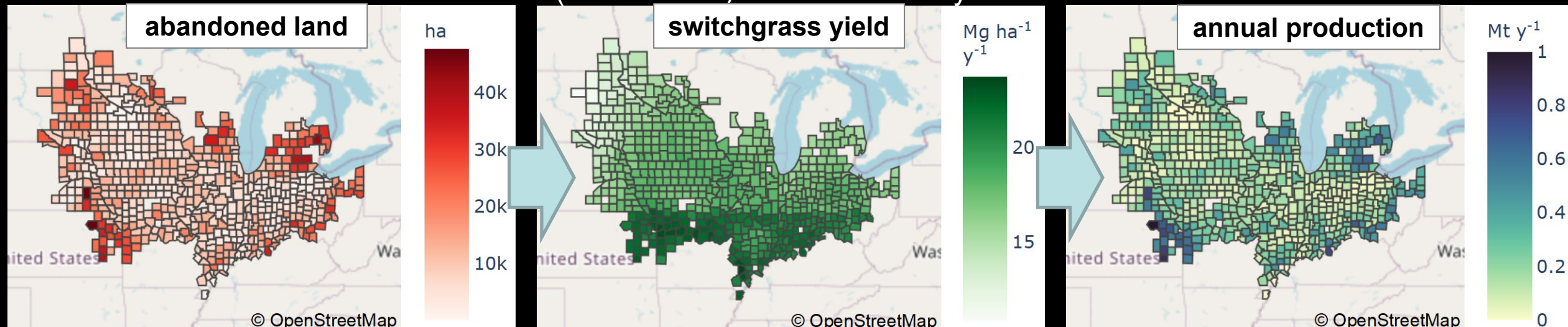
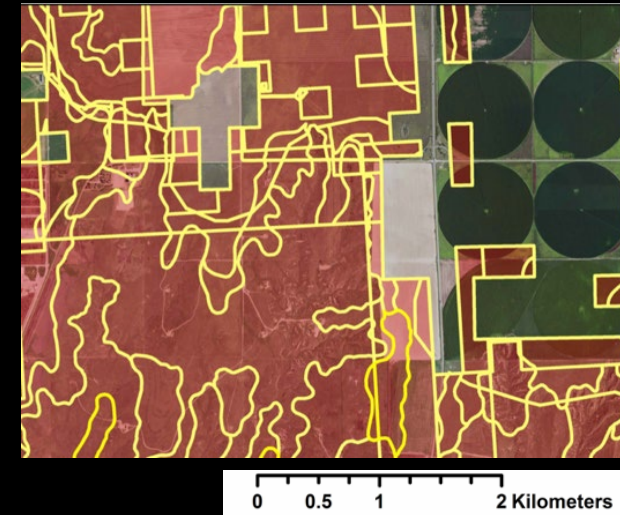
Spatially-resolved data generated from DayCent model

- Process-based simulation of **crop yields**, **soil carbon changes**, other **soil GHG emissions** as affected by soil, climate, and land management

Python-based spatial modeling workflow:

1. Identification of target **land base** (e.g., existing annual cropland, marginal or abandoned land, etc.)
2. Specification of **management scenarios** (e.g., fertilizer application rates, stover removal, etc.) & associated **pseudo field-scale model runs**
3. Automated simulation execution (CSU cluster) and results analysis

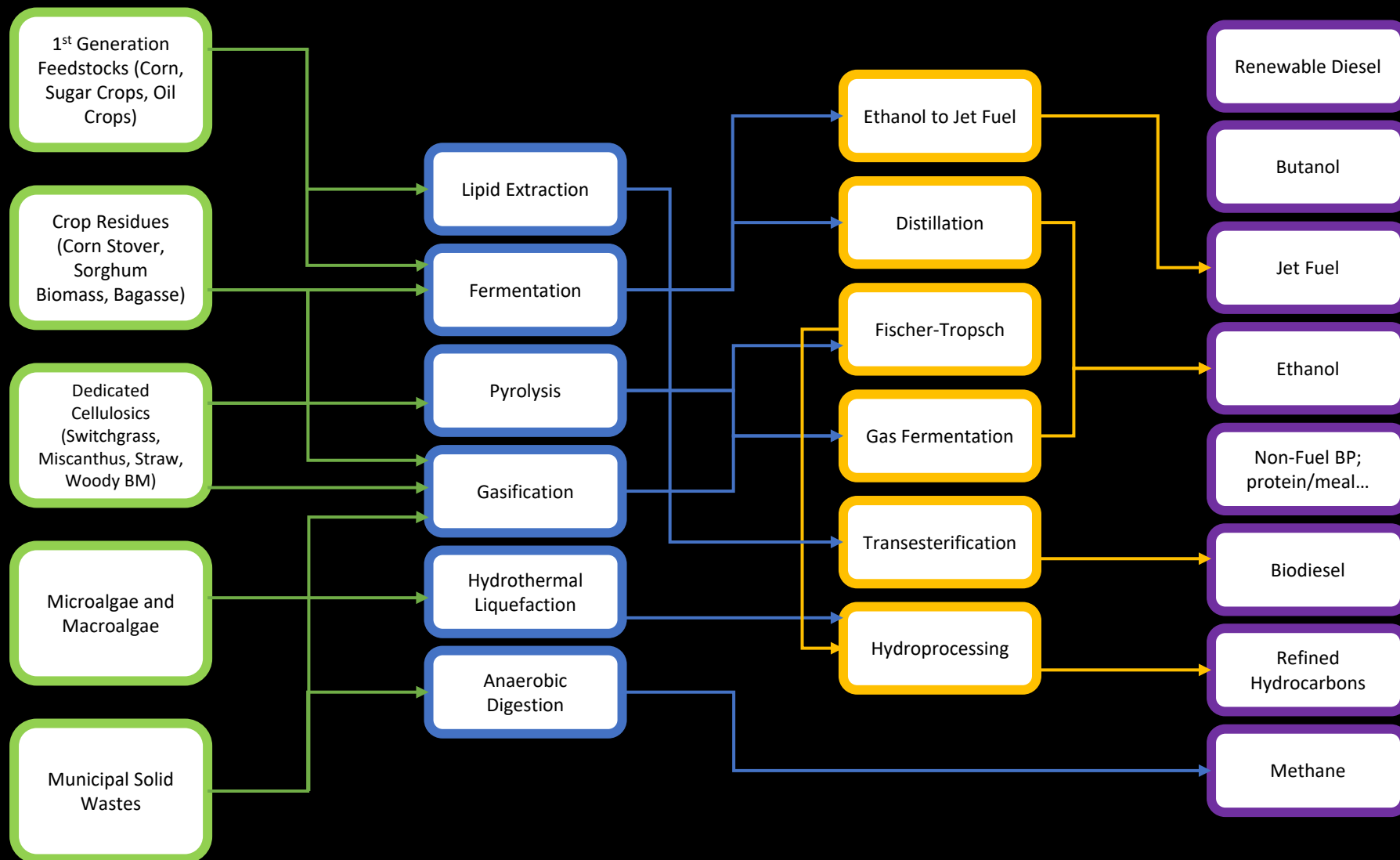
pseudo field-scale simulation



2 – Approach

Modular Process Modeling

Fundamental Process Models



Numerous Pathways – Consistent Methodology

Defines Potential Solution Space (Enables Project)

LCA and TEA Results
MFSP
Greenhouse Gas Impact
Water Use
Criteria Pollutants

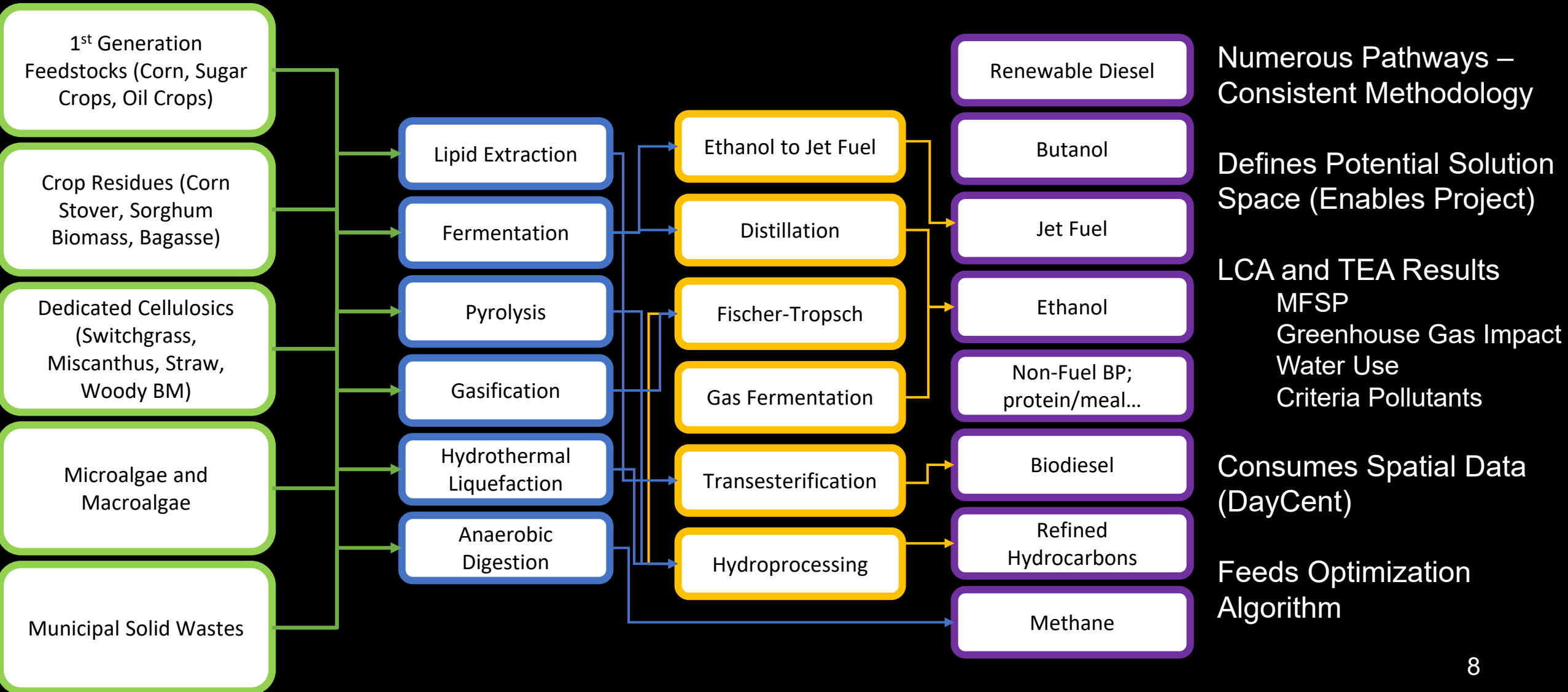
Consumes Rich Spatial Data (DayCent)

Feeds Optimization Algorithm

2 – Approach

Modular Process Modeling

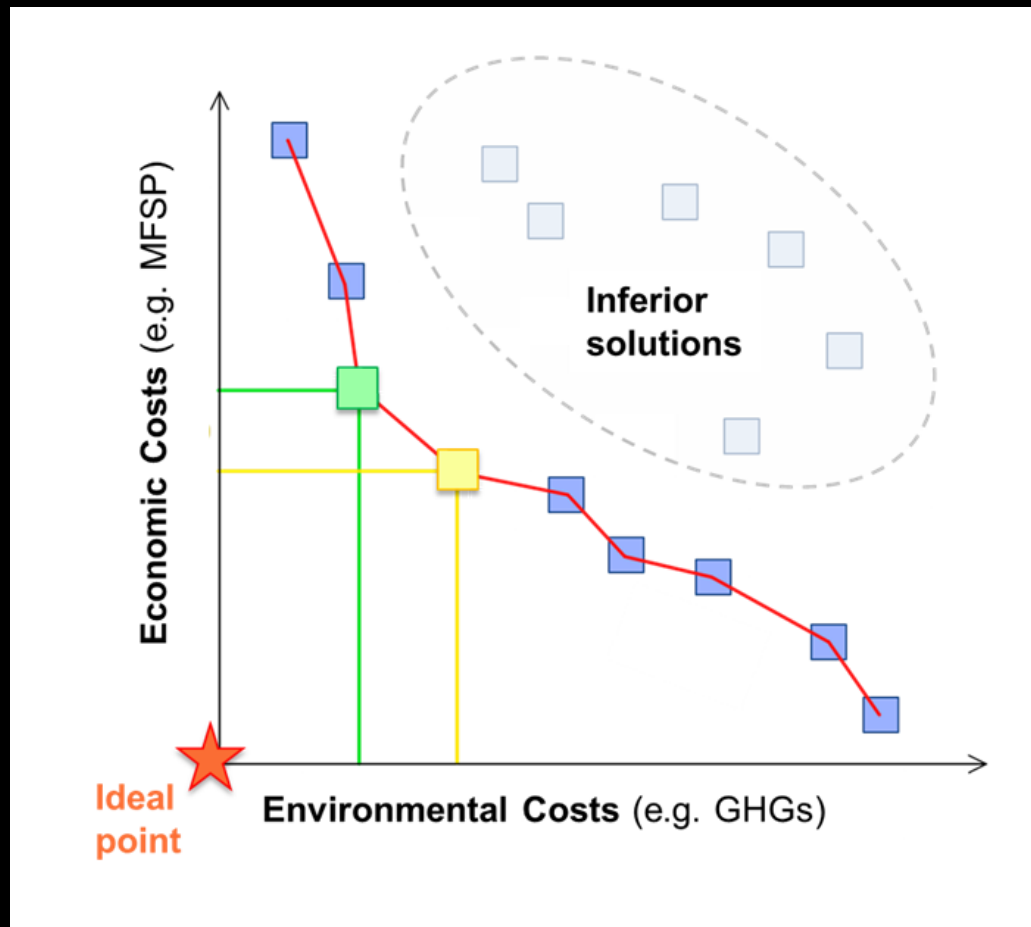
Fundamental Process Models



2 – Approach

Multi-objective Optimization

Embed LCA/TEA within Multi-objective optimization of Biofuel Supply Chain (farm to fuel)



■ = 1 Viable Supply Chain Network

Optimize County-to-Hub Supply Chain Network

Decision variables:

- County level cultivation choices (feedstock, volume)
- Flow of biomass between preprocessing hubs and biorefineries
- Biorefinery design, size and location
- End product choice

Constraints:

- Production quotas, resource usage (land, water), supply vulnerability (weather)

Navigating Tradeoffs in Cost and Greenhouse Gas Emissions (what if there's no silver bullet?)

Better understand design choices that lead to:

■ Higher cost + lower emission

vs

■ Lower cost + higher emission

2 – Approach

Agent Based Modeling

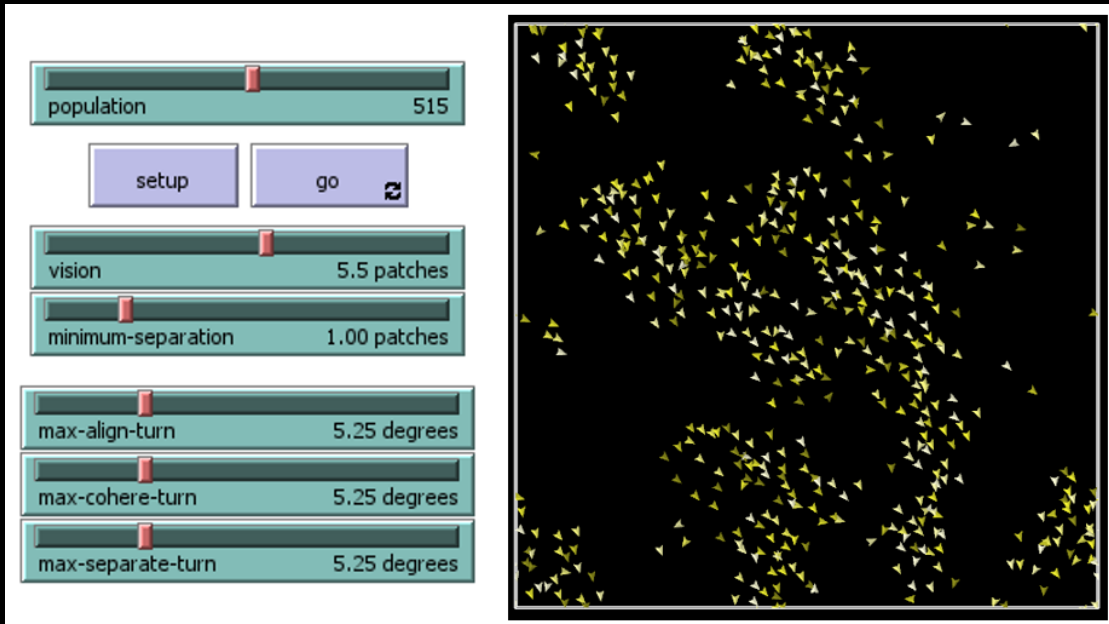
Agents in US Bioeconomy

Framework Capacity:

- Farmer/Biorefinery/Consumer Interaction and Behavior
- Predict Pathway Adoption Rates and Mechanisms
- Identification of Levers in Industry
- Informs Behavior of Proposed Policy

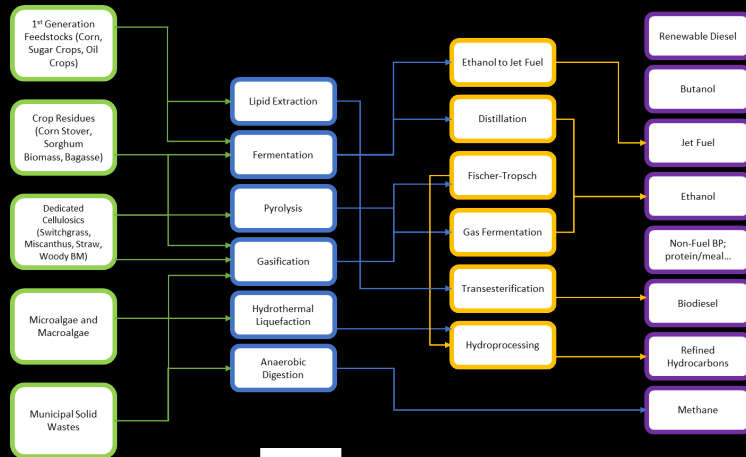
Characteristics:

- Yearly Time-Steps (Analysis of Intermediate States)
- Preserves Heterogeneity
- Potential to Model Adaptive Behavior

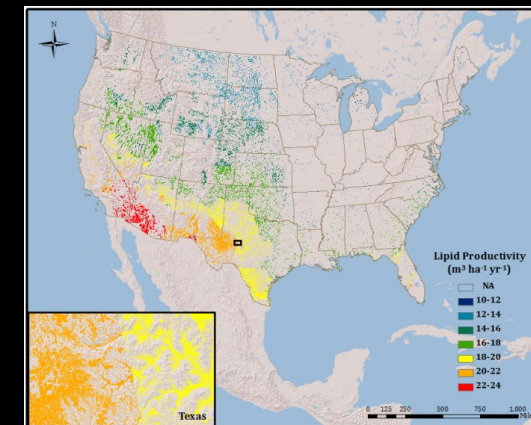


2 – Approach Future Work

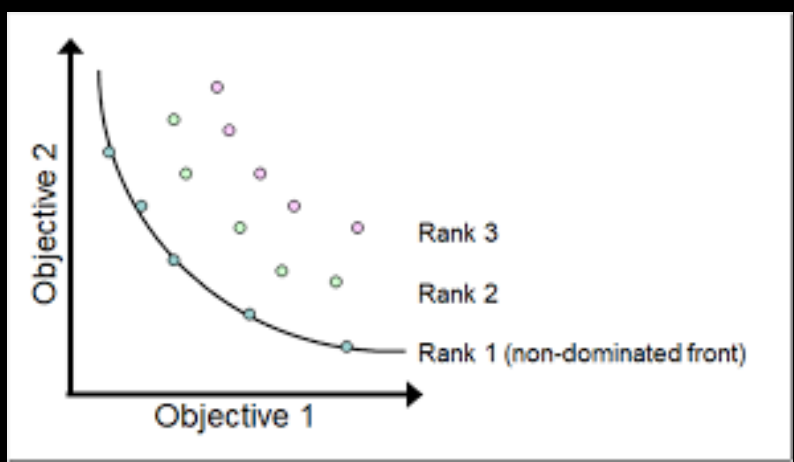
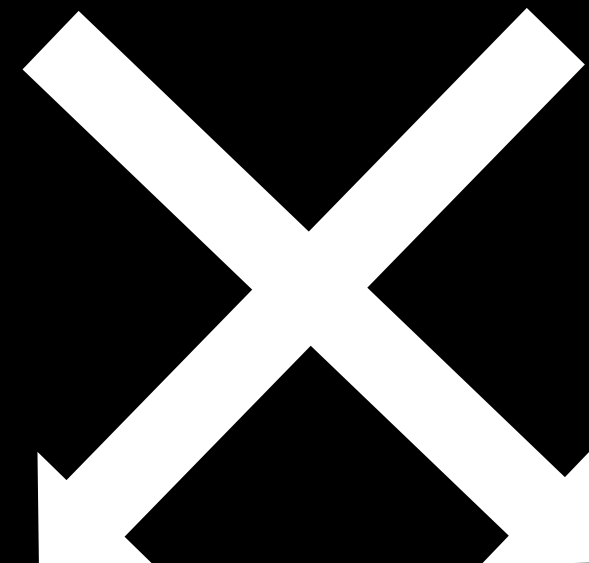
Expanding Process Modeling Pathways



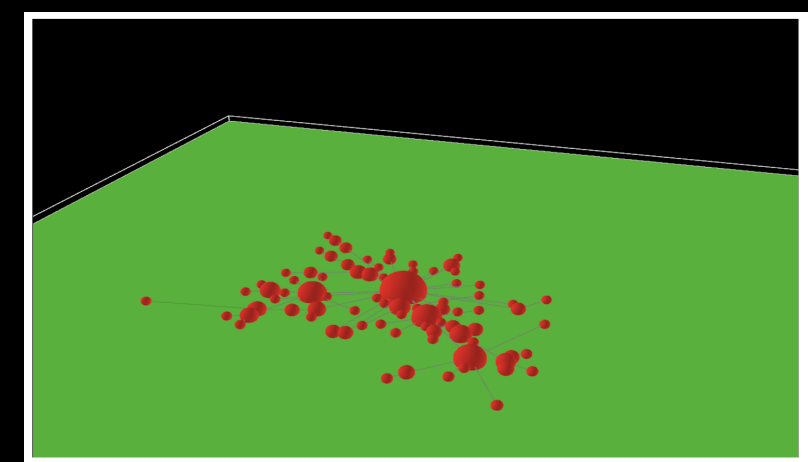
Continued Geospatial Modeling



US Policy



Multi-objective Optimization



Agent Based Modeling

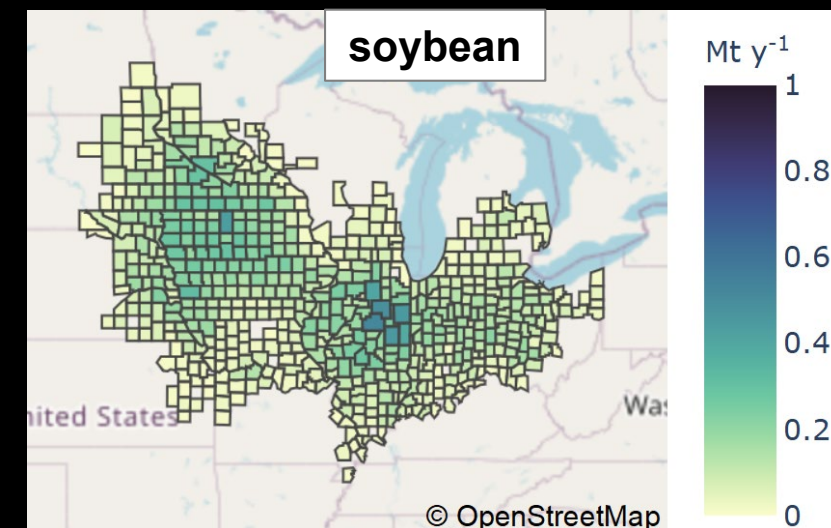
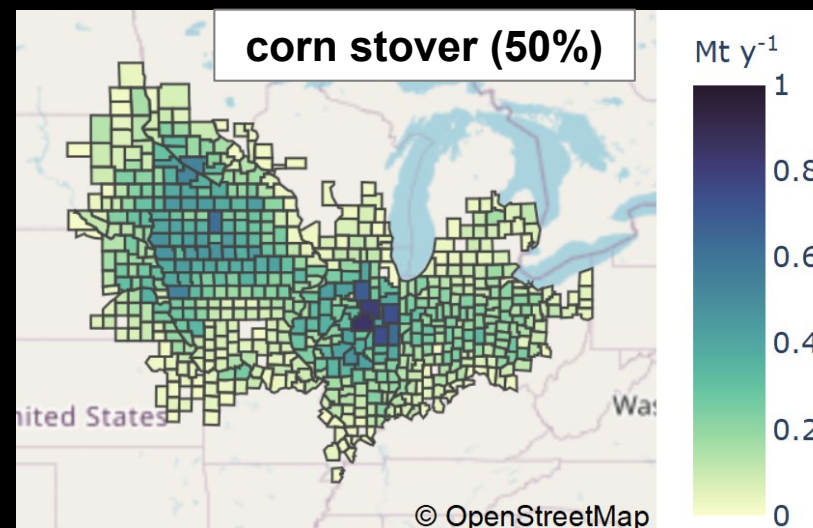
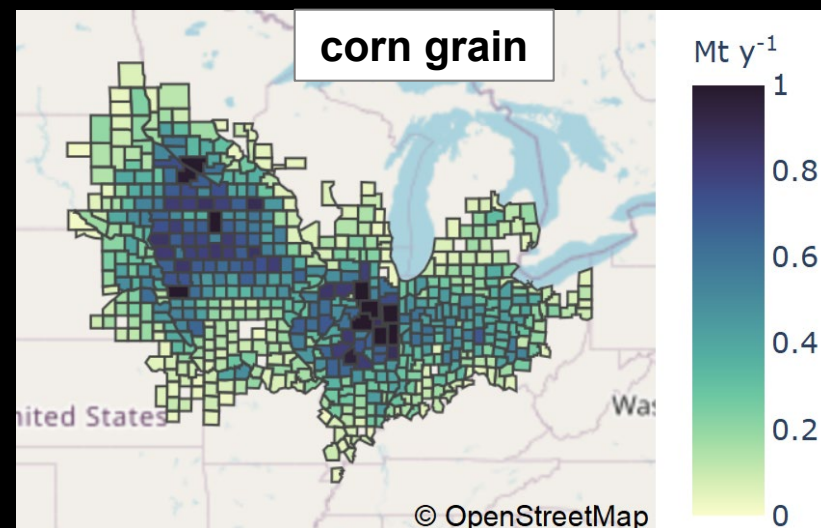
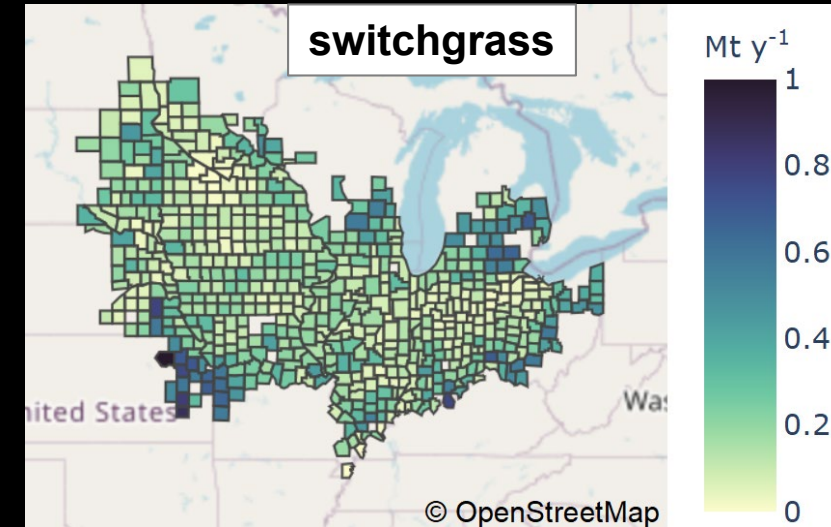
3 – Impact

- *Goal of the project is IMPACT*
 - *Identifying technologies and pathways that meet DOE sustainability targets*
 - *Identify performance (R&D) targets for DOE and Industry*
- *System level assessment*
 - *Not individual technologies*
- *Department of Energy is Dynamic*
 - *Modeling work is intended to be re-active and adjustable*
 - *Current administration is focusing on the environment*
 - *Future of biofuels (heavy fuels and jet)*
- *Generation of open-source toolset*

4 – Progress and Outcomes

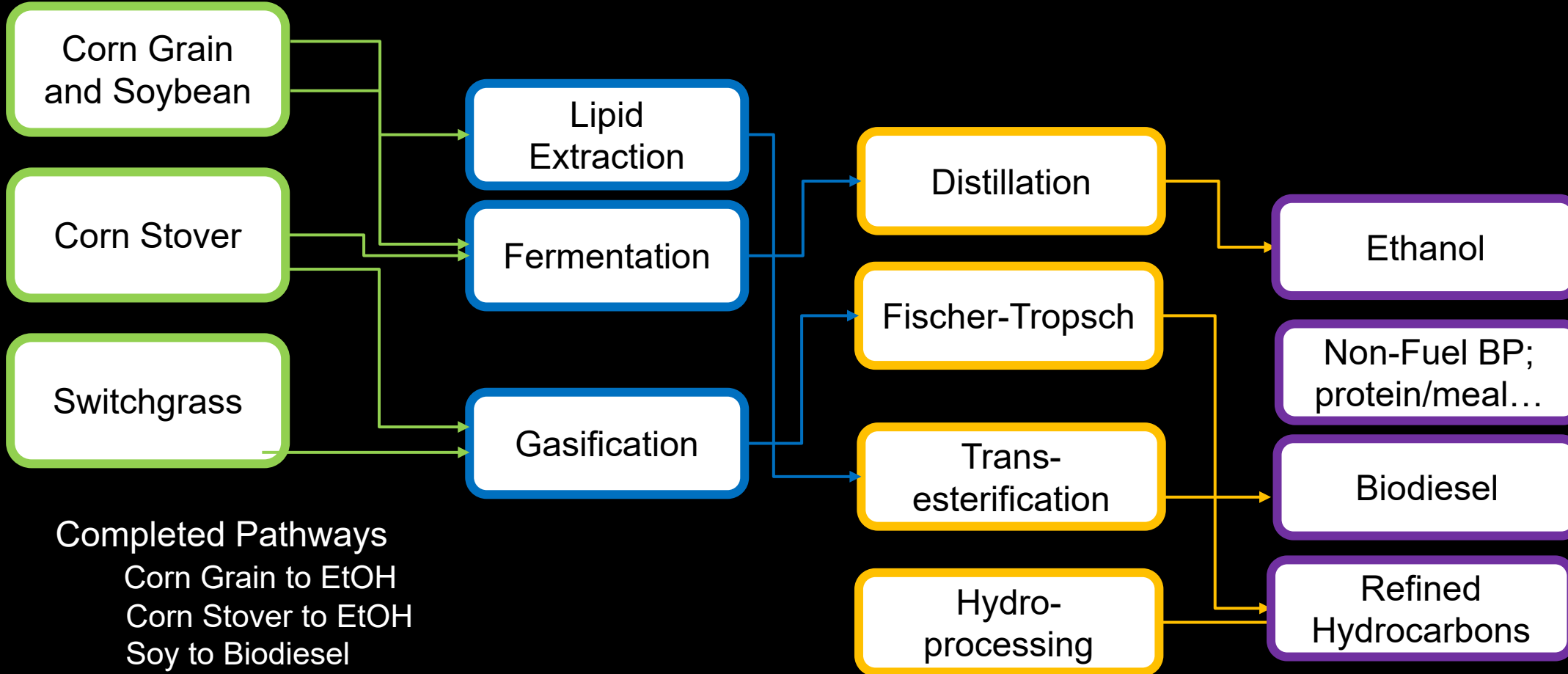
DayCent: Geospatial Agricultural Modeling

- Completed curation of modeling results for current-day **corn–soybean** cultivation in US Corn Belt, incl. **stover harvest**
 - Highest density of production in Iowa, Illinois
 - Quantified soil carbon penalty of different rates of stover harvest rates
- Preliminary results for **switchgrass** cultivation on **abandoned cropland** across same region
 - Abandoned land down-scaled from historical county land use records
 - Different spatial pattern, with abandoned land most concentrated at periphery of the Corn Belt
 - Ongoing modeling effort to capture baseline for business-as-usual management of abandoned lands



4 – Progress and Outcomes Process Modeling

Process Modeling



Completed Pathways

- Corn Grain to EtOH
- Corn Stover to EtOH
- Soy to Biodiesel
- Switchgrass to Jet
- Corn Stover to Jet

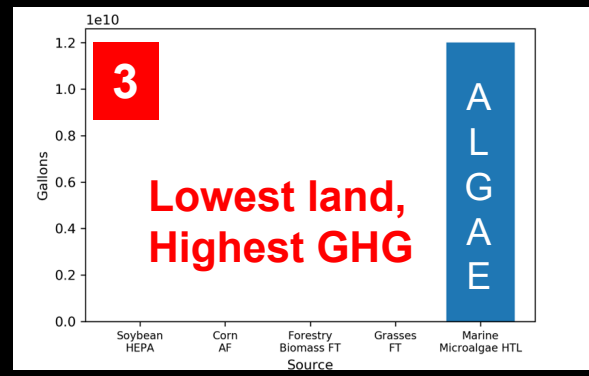
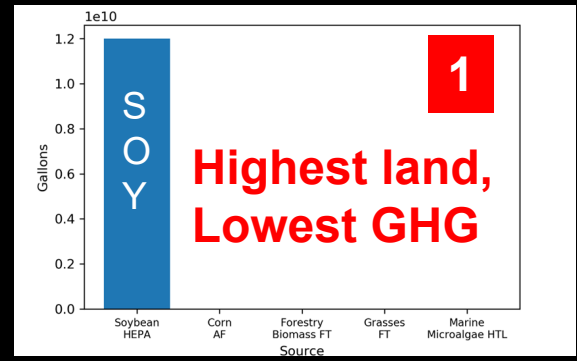
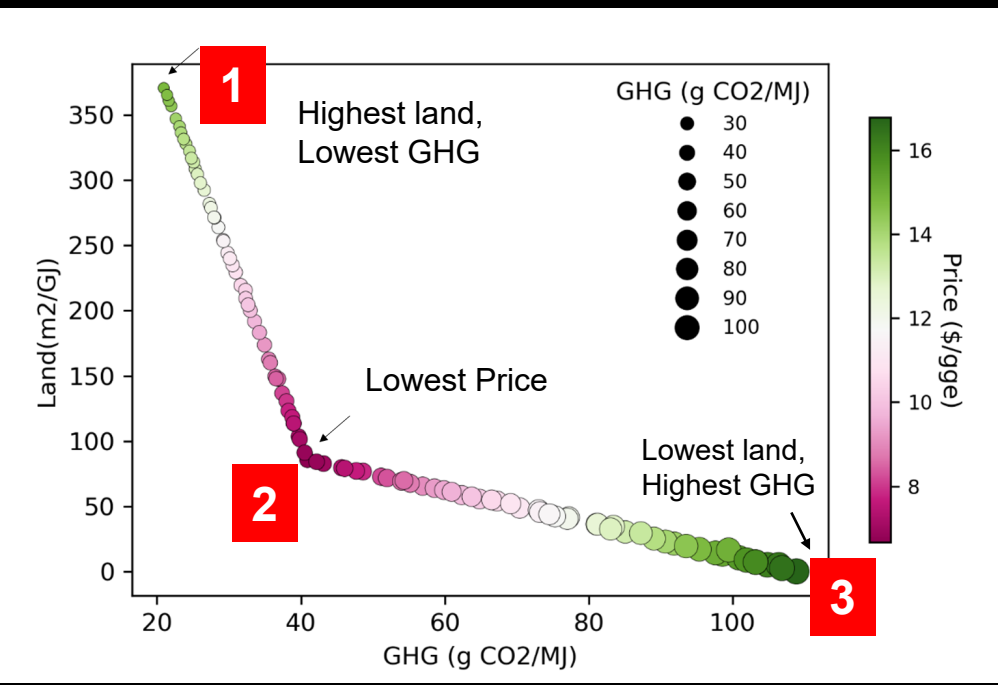
Flexible Structure – Facilitates Added Pathway Steps

4 – Progress and Outcomes Multi-objective Optimization

Multi-objective optimization of Biofuel Supply Chain (farm to fuel)

Initial proof-of-concept for 5 national jet fuel pathways: Balance cost, GHGs, and land use, produce 12M gallons

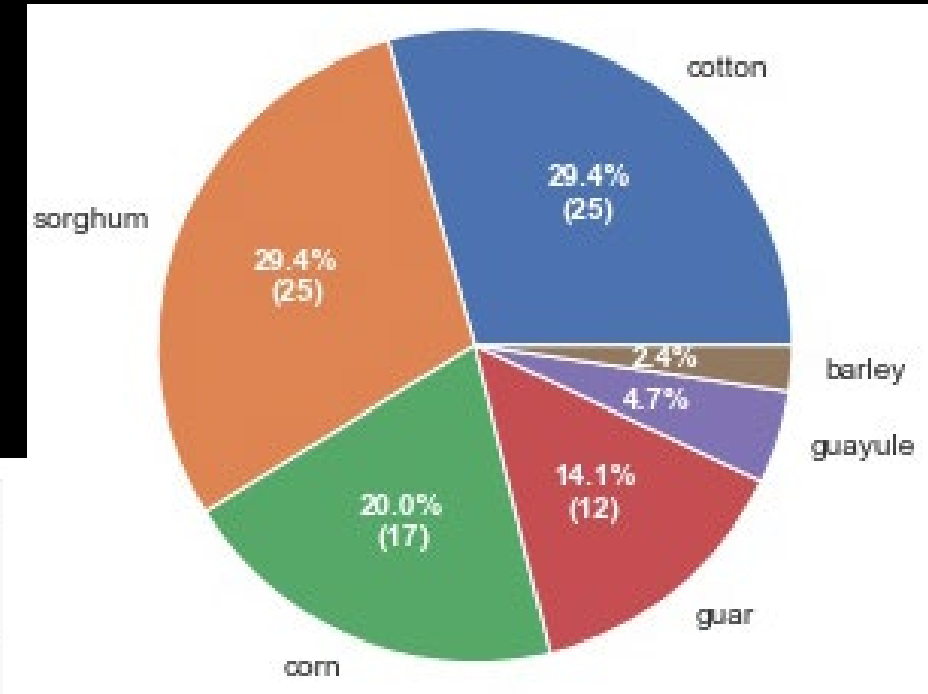
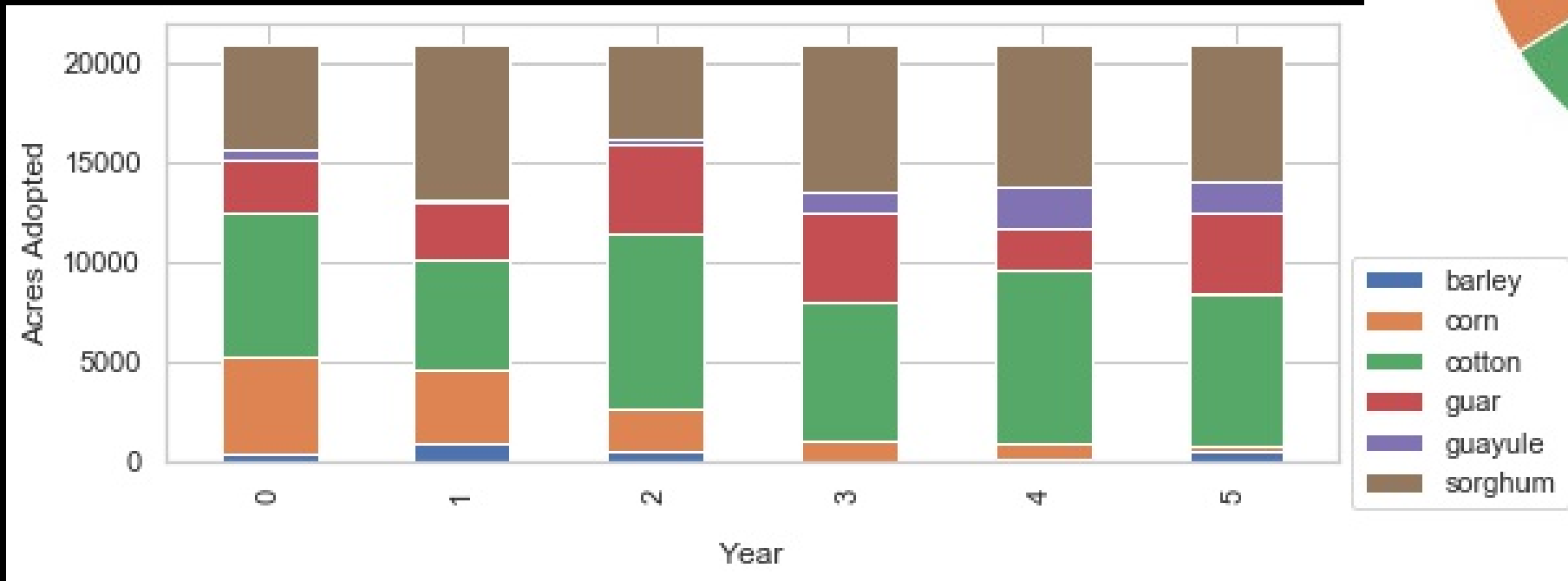
| Source | Cost (\$/gge) | Post-Combustion GHG (g CO2e/MJ) | Arable Land (m2/GJ/yr) | Nitrogen (g/GJ) |
|-----------------------|---------------|---------------------------------|------------------------|-----------------|
| Soybean HEFA | \$14.85 | 20.94 | 370.75 | 102.08 |
| Corn AF | \$6.66 | 40.92 | 85.52 | 1,186.38 |
| Forestry Biomass FT | \$7.11 | 70.88 | 99.64 | 354.82 |
| Grasses FT | \$8.24 | 41.87 | 128.17 | 1,512.40 |
| Marine Microalgae HTL | \$16.79 | 108.90 | 0.00 | 226.60 |



4 – Progress and Outcomes Agent Based Modeling

Scenarios:

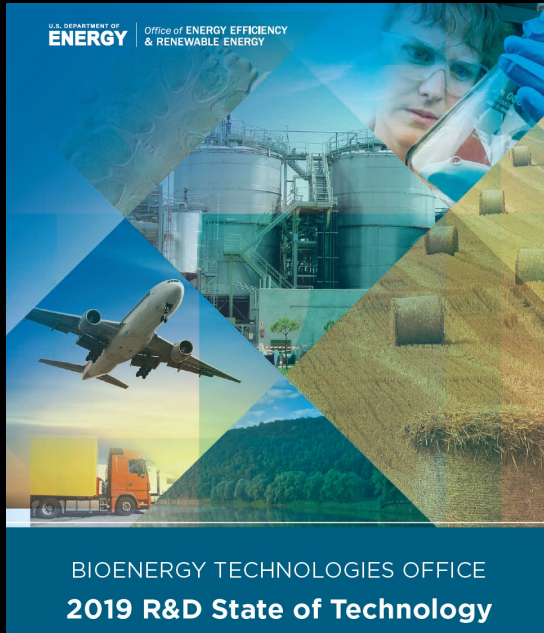
- 1) Only profitability
- 2) Only familiarity
- 3) Only environmental
- 4) **Equal weighting**
- 5) Random weighting



4 – Progress and Outcomes Future Direction

Near Term

Compliment and Add to the DOE



Note future potential

- >1 billion tons biomass in 2040
- ~35% from dedicated energy crops

Identify promising case studies

Long Term

Integrated Assessment Model

- Dynamic assessment tool
- Holistic tool set that investigates non-trivial trade-offs
- Enables informed policy decisions
- Leverages multiple optimization techniques

Open-source model for the community

4 – Progress and Outcomes

| | |
|-----------------|---|
| 1 | Development of modular engineering process models |
| 2.0 | Development of concurrent and spatially explicit sustainability models |
| 3.0 | External Review |
| Go/No-go | Modeling of 6 production pathways with results quantifying water consumption, energy consumption, greenhouse gas emissions, and pollutant emissions for fuel products on the metrics of MJ MJ-1, g-CO ₂ -eq MJ-1, and g MJ-1, respectively |
| 4.0 | Development of modular engineering process models |
| 5.0 | Optimization and evaluation of favorable configurations |
| 6.0 | External review |

Progress:

- On schedule with process modeling
- Ahead of Schedule on optimization work

Summary

- *Demonstrated capabilities*
- *Adapting to Directions of the DOE*
- *Established an effective working team*
- *Technical achievements*
 - *Modular Process modeling*
 - *Demonstrated proof of concept on MOO and ABM*
 - *Geospatial data modeling and integration*
- *Defining near term directions with the DOE*

Quad Chart Overview

BETO FY19 Multi-Topic FOA, AOI 10: Reducing Water, Energy, and Emissions in Bioenergy.

Timeline

- 10/01/2019
- 09/30/2021

| | FY20 Costed | Total Award |
|---------------------------|---|-------------|
| DOE Funding | (10/01/2019 – 9/30/2020) \$15,703.51 | \$1,000,000 |
| Project Cost Share | \$250,000 | |

Project Partners*

- North Carolina State University
- B&D Consulting

Project Goal

Develop an open-source sustainability model that supports the strategic investment of research by the DOE to achieve renewable fuel goals.

End of Project Milestone

- Develop an open source bioenergy tool to support strategic investments by DOE.
- Identify optimum bioenergy pathways through Agent Based Modeling (ABM) and multi-objective optimization to meet sustainability goals: reduction in water consumption, energy consumption, greenhouse gas emissions, and/or pollutant emissions.
- Couple economic modeling and life cycle assessment to understand the impact of carbon accounting on technology investments.

Funding Mechanism

DE-FOA-0002029

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