NETL - Penn State

University Coalition for Fossil Energy Research

2021 UCFER TECHNICAL REVIEW MEETING

CURRENT STATUS OF DOE-NETL UNIVERSITY COALITION FOR FOSSIL ENERGY RESEARCH

BRUCE G. MILLER

DOE Award Number: DE-FE0026825

Period of Performance:10/01/2015 - 06/30/2023

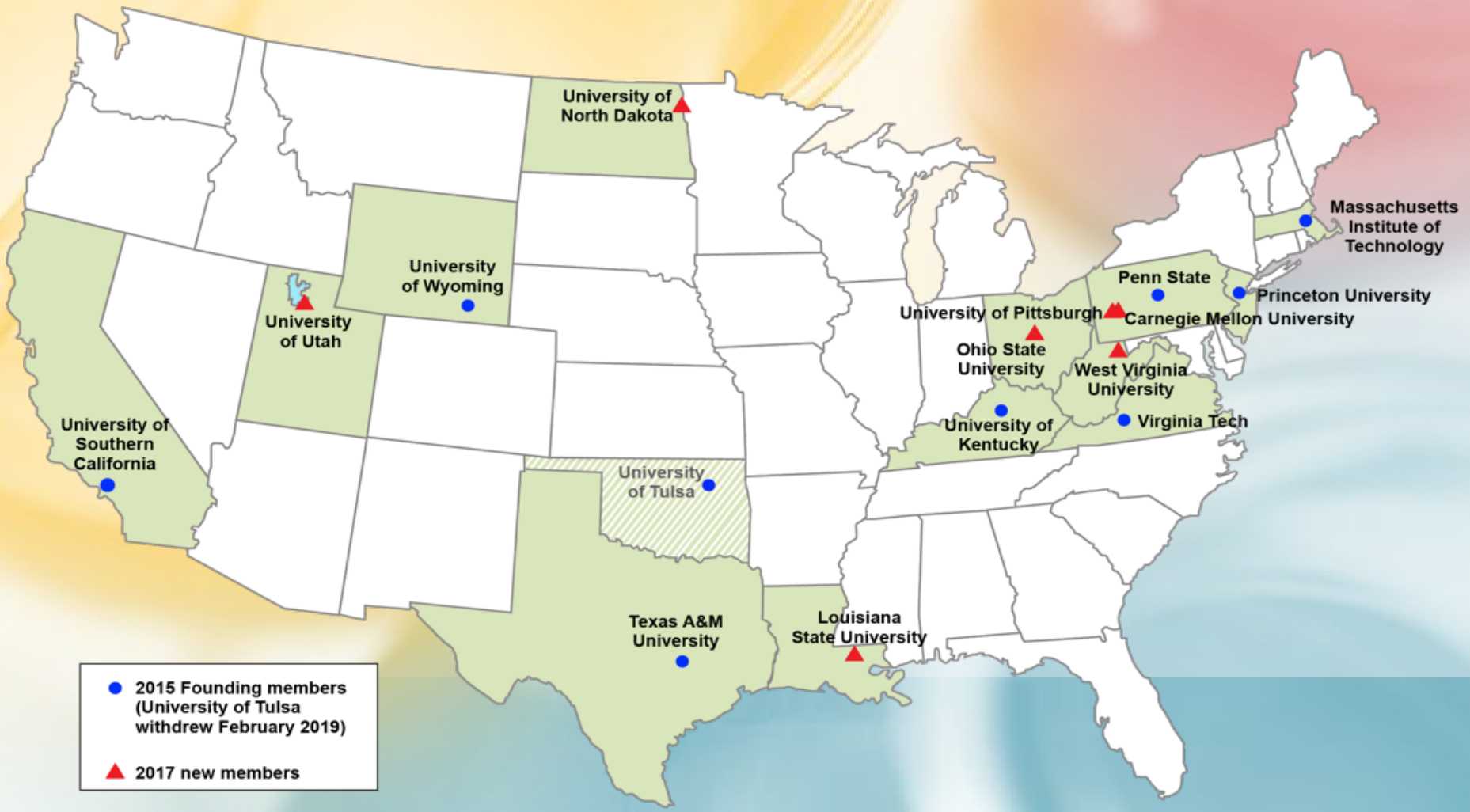
PRESENTATION OUTLINE

- Background of UCFER
- UCFER Organizational Structure
- Research Focus
- Research Funding and Status
  - Summary of six rounds of solicitations and projects selected
- Collaboration with NETL
- Impact of UCFER Program
  - Participants, products, impact on energy development technology, collaborations
- Outreach Activities
- Acknowledgements

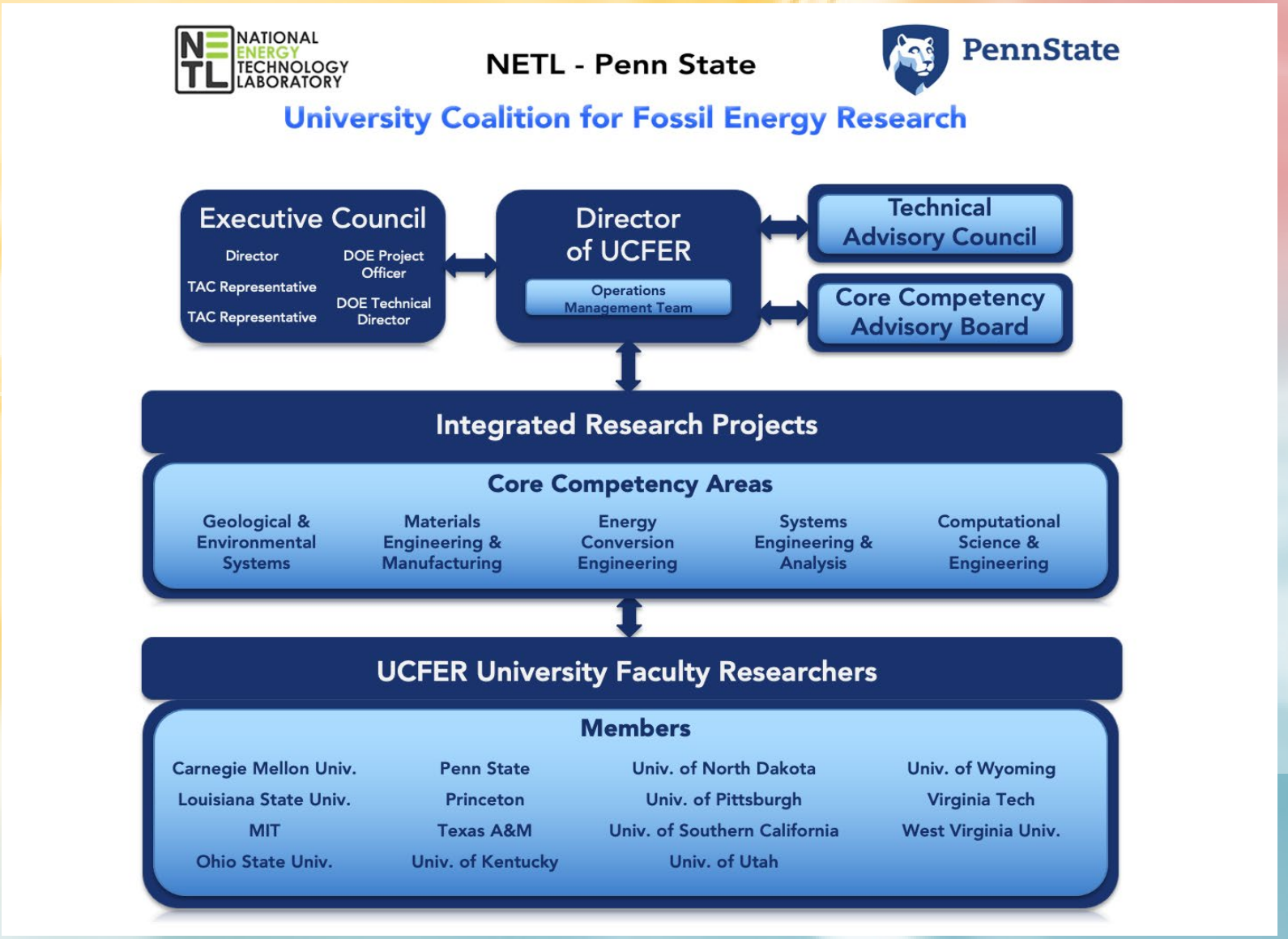
BACKGROUND

- UCFER was established in 2015 following a nationwide open competition
- Penn State led a team of 9 universities; 7 more universities added in 2017
- Goals: To advance basic and applied energy research and to promote university/NETL collaboration for more efficient and more environmentally friendly utilization of coal, oil, and natural gas for fuels, chemicals, and materials.
- Objectives: UCFER will identify, select, execute, review, and disseminate knowledge from university-based research that will improve the efficiency of production and use of fossil energy resources while minimizing the environmental impacts, reducing greenhouse gas emissions including carbon capture, storage, and utilization, and advancing the production of value-added chemicals and materials from fossil resources.
- Details on UCFER organizational structure and operation can be found at https://sites.psu.edu/ucfer/

UCFER UNIVERSITIES



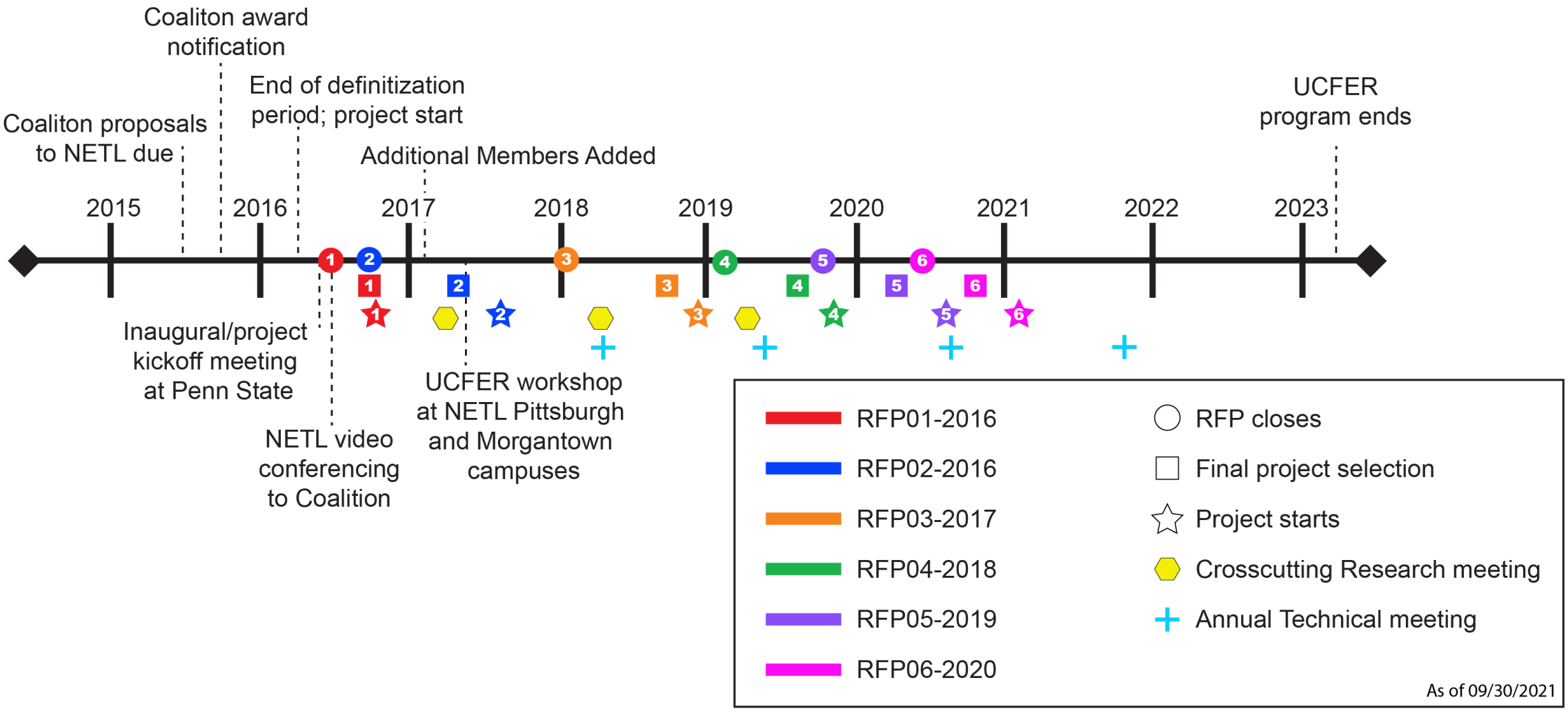
UCFER ORGANIZATION CHART



TAC AND CCAB MEMBERS

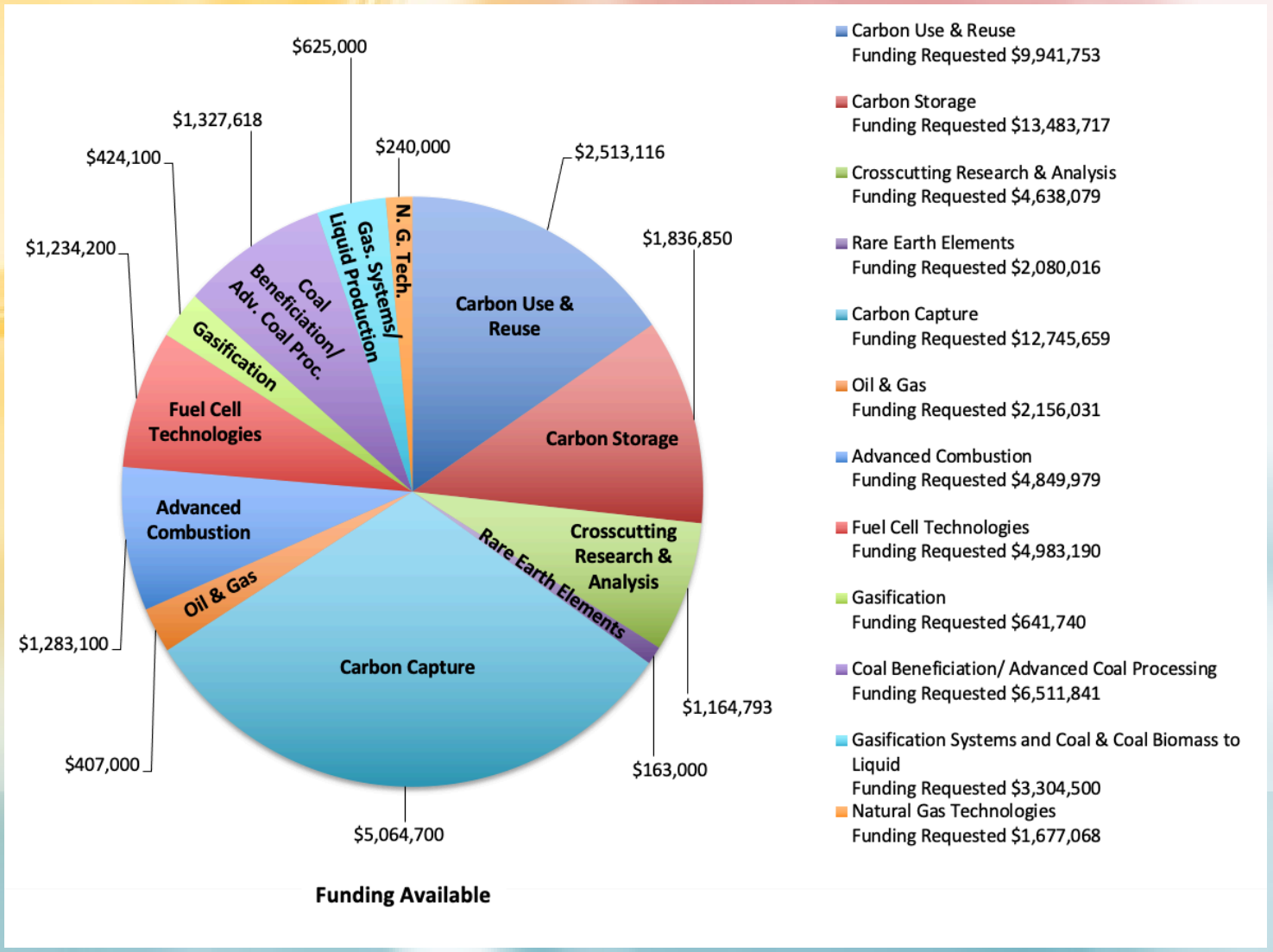
University	TAC Member	CCAB Member
Carnegie Mellon University	Andrew Gellman	Nicholas Z. Muller
Louisiana State University	James Spivey	Ye Xu
Massachusetts Institute of Technology	Bradford Hager	Ruben Juanes
Princeton University	Yiguang Ju	Claire White
Texas A&M University	Stratos Pistikopoulos	Hong-Cai (Joe) Zhou
The Ohio State University	David Cole	Andrew Tong
The Pennsylvania State University	Bruce Miller	Adri Van Duin
University of Kentucky	Rodney Andrews	Rick Honaker
University of North Dakota	Michael Mann	James A. Sorensen
University of Pittsburgh	Götz Veser	Chris Wilmer
University of Southern California	Kristian Jessen	Theo Tsotsis
University of Utah	Arnis Judzis	Kevin J. Whitty
University of Wyoming	Richard Horner	David Bell
Virginia Tech	Roe-Hoan Yoon	Changmin Son
West Virginia University	Richard A. Bajura	Debangsu Bhattacharyya

UCFER TIMELINE OF MAJOR ACTIVITIES



RESEARCH FUNDING THROUGH 6 ROUNDS OF SOLICITATIONS

- 12 topic areas funded
- $16.6 M funding available
- 259 proposals submitted
- $67.0 M funding requested
- 43 projects awarded



SUMMARY OF PROPOSALS SUBMITTED AND FUNDED

Solicitation Round	Funding Available ($M)	No. of Proposals Submitted	No. of Projects Funded	Success Rate (%)
Round 01	1.9	39	6	15.4
Round 02	2.1	25	6	24.0
Round 03	4.1	81	11	13.6
Round 04	1.9	41	6	14.6
Round 05	2.8	37	7	18.9
Round 06	3.8	36	7	19.4
Total	16.6	259	43	16.6

ADDITIONAL PROPOSALS/PROJECTS ANALYTICS

Technology Line	No. of Proposals Submitted	No. of Projects Funded
Carbon Use & Reuse	31	4
Carbon Storage	54	6
Crosscutting Research & Analysis	17	4
Rare Earth Elements	13	1
Carbon Capture	52	12
Oil & Gas	5	1
Advanced Combustion	15	4
Fuel Cell Technologies	23	4
Gasification	2	1
Coal Beneficiation/Advanced Coal Processing	25	3
Gasification Systems and Coal & Coal Biomass to Liquid	10	2
Natural Gas Technologies	8	1
Carbon Utilization	4	0
Total	259	43

RFP 01: $1.9M FUNDING AVAILABLE, $7.7M FUNDING REQUESTED, 39 PROPOSALS

Area	PI	Title	Progress
Carbon Storage	F. Aminzadeh/USC	Integration of Geophysical and Geomechanical Modeling	Completed
	S. Yin/UWy	A Low-Cost Technique for In-Situ Stresses and Geomechanical Properties Measurement Based on Leak-Off Tests and Caliper Logs	Completed
Carbon Use & Reuse	B. Koel/Princeton	Converting CO_2 and Methane to Fuels by Enhanced Plasmonic Effects in a Nanotemplated Catalyst Plasma Reactor	Completed
	M. Hickner/PSU	Efficient Reduction of CO_2 in a Bipolar Electrochemical Cell	Completed
Crosscutting Research & Analysis	A. Ghoniem/MIT	Grid Independence and Uncertainty Quantifications in Gas-Solid Flow Simulations	Completed
	B. Jafarpour/USC	A Novel Point Process Paradigm for Stochastic Modeling and Inversion of Microseismic Monitoring Data for CO_2 Storage	Completed

RFP 02: $2.1M FUNDING AVAILABLE, $8.2M FUNDING REQUESTED, 25 PROPOSALS

Area	PI	Title	Progress
Advanced Combustion	E. Petersen/TAMU	CFD Model Development for Direct Fired Supercritical CO_2 Power Cycles	Completed
	S. Pisupati/PSU	Evaluation of Agglomeration Potential of Oxygen Carriers for Chemical Looping Combustion (CLC) and Chemical Looping with Oxygen Uncoupling (CLOU)	Completed
	R. Yetter/PSU	Fundamental Studies on the Reaction Mechanisms of Oxygen Carriers for CLC/CLOU of Solid Fuels	Completed
Carbon Capture	B. Wilhite/TAMU	Layer-by-Layer Functional Thin Film Coatings for Enhanced Light Gas Separations	Completed
	M. Hickner/PSU	Innovative Polymeric Membrane Materials for Separation of CO_2/N_2	Completed
Oil & Gas/NG Infrastructure	N. Ripepi/VT	Methane Emissions Quantification (MEQ) of Compressor Stations	Completed

RFP 03: $4.1M FUNDING AVAILABLE, $20.2M FUNDING REQUESTED, 81 PROPOSALS

Area	PI	Title	Progress
Advanced Combustion	R. Miles/TAMU	Seed-Free MHD Topping Cycle for Coal and Gas-Fired Power Generation	Completed
Carbon Capture	N. Rosi/UPitt	Modular Chemical Functionalization of External Surfaces of Porous Metal-Organic Framework for Filler Particles for Optimization of Interfacial Properties in Mixed Matrix Membranes	Completed
	H.-C. Zhou/TAMU	Porous Polymer Network Membranes with Porous Molecular Additives for Post-Combustion CO_2 Capture	Completed
	G. Krishnamoorthy/UND	A Multiphase Modeling Framework for Second Generation Post-Combustion Carbon Capture Systems	Completed
Carbon Storage	R. Enick/UPitt	Novel Wellbore Cementing Materials for Long-Term Containment Assurance	Completed
	B. Jafarpour/USC	CO_2 Storage Optimization under Geomechanical Risk and Prediction Uncertainty Using Coupled-Physics Models	Completed
Carbon Use & Reuse	J. Spivey/LSU	Catalytic Conversion of CO_2 into Vinyl Acetate	Completed
	G. Mpourmpakis/UPitt	Atomically Precise Au25-Based Alloy Nanoclusters for Electrochemical CO_2 Conversion	Completed
Fuel Cell Technologies	R. Vander Wal/PSU	Optimization of Microwave-Driven, Plasma-Assisted Conversion of Methane to Hydrogen and Graphene	Completed
	H. Tian/WVU	Autothermal Methane Decomposition for Large-Scale Co-production of CO_2-free H_2 and Alinged Carbon Nanotube	Completed
Gasification	T. Musho/WVU	Computational Investigation of Coal Conversion via Microwave Induced Plasmas	In Progress

RFP 04: $1.9M FUNDING AVAILABLE, $10.6M FUNDING REQUESTED, 41 PROPOSALS

Area	PI	Title	Progress
Carbon Storage	C. Chen/VT	Upscaling Experimental Measurements to the Field Scale Using a Machine-Learning-Based, Scale-Bridging Data Assimilation Approach	In Progress
Coal Beneficiation	R. Qiao/VT	Developing a Novel Ultrafine Coal Dewatering Process	Completed
	X. Hou/UND	Porous Silicon/Lignite-Derived Graphene Composite Anodes for Lithium-Ion Batteries	In Progress
Crosscutting Research	E. Holm/CMU	Computer Vision and Machine Learning Making the Processing-Microstructure-Property Connection in Heat Resistant Alloys	In Progress
Fuel Cell Technologies	Y. Ju/Princeton	Development of a Novel Supersonic Hybrid Non-equilibrium Plasma Reactor for Efficient and Tunable Co-Production of Hydrogen and Value-Added Solid Carbons	In Progress
	R. Vander Wal/PSU	Metal-free Catalyzed Synthesis of Novel Carbon by Carbon Allotrope Seeds	In Progress

RFP 05: $2.8M FUNDING AVAILABLE, $10.9M FUNDING REQUESTED, 37 PROPOSALS

Area	PI	Title	Progress
Carbon Capture	A. Morris/VT	Development and Optimization of Metal Organic Framework (MOF) Sorbents for Direct Air Capture (DAC) of CO_2	In Progress
	K. Hornbostel/UPitt	Core-Shell MOFs for Direct Air Capture	In Progress
	H.-C. Zhou/TAMU	Selective Porous Polymer Networks Supported on Hollow Fiber Superstructures for Direct Air Capture of CO_2	In Progress
Gasification Systems and Coal Biomass to Liquids	J. McKone/UPitt	A Novel Modular Coal-to-Methanol Reactor Using Electroactive Membranes	In Progress
	M. Nigra/Utah	Design of Bifunctional Structured Fischer-Tropsch Catalysts with Improved Heat Conductivity for Modular Small-Scale Reactor Applications	In Progress
Natural Gas Technologies	A. Presto/CMU	Quantification of Methane Emissions from the Natural Gas Gathering System Using Distributed Sensors	In Progress
Rare Earth Elements	R. Vander Wal/PSU	Current Users and Future Opportunities for US Industry in Rare Earth Elements and Critical Minerals Technologies and Markets: Knowledge-Base Tool Development	In Progress

RFP 06: $3.8M FUNDING AVAILABLE, $11.5M FUNDING REQUESTED, 36 PROPOSALS

Area	PI	Title	Progress
Crosscutting Research	M. Mueller/Princeton	Adaptive Depth Neural Networks for Scale-Bridging Modeling of Multiphase Reacting Flows	Started 3/3/21
	W. Xiong/UPitt	Wire Arc Additive Manufacturing of Advanced Steam Cycle Components Using Location Specific Design Enhanced by High-Throughput Experiments and Machine Learning	Started 2/9/21
Advanced Coal Processing	H. Tian/U Kentucky	UCFER-An Economically-Viable Technology for Production of Coal-Derived Aerogel Insulation Envelope	PI moved from WVU to UK; subcontract not executed
Carbon Capture	X. Hou/UND	Crosslinked Microspherical Adsorbents from Lignite-Derived Humic Acid for CO_2 Capture	Started 4/9/21
	B. Irvin/U Kentucky	Development of Novel Process Intensification Device, Acoustic Driven Packing Material	Started 1/7/21
	T. Tsotsis/USC	A Novel Reactive Separation Method for Carbon Dioxide Capture from Flue Gas	Started 1/12/21
	M. Fan/U Wyoming	Use of a Novel Process for Revolutionizing CO_2 Capture	Started 2/9/21

STATUS OF FUNDED PROJECTS

- Round 01 Projects – All 6 projects completed
- Round 02 Projects – All 6 projects completed
- Round 03 Projects – 10 projects completed; 1 project to be completed late fall 2021
- Round 04 Projects – 1 project completed; 4 projects to be completed late 2021; 1 project to be completed in 2022
- Round 05 Projects – 7 projects ongoing, to be completed mid 2022
- Round 06 Projects – 6 projects just started, 1 project not started yet, all must be completed early-to-mid 2023

- Totals: 23 projects completed; 19 projects ongoing; 1 project yet to begin

UNIVERSITY COLLABORATION IN PROPOSALS

Solicitation Round	Topic Area	Lead University	Subcontracting University
1	Carbon Use & Reuse	USC	Wyoming
	Carbon Storage	Penn State	Wyoming
2	Advanced Combustion	Princeton	Penn State
		Penn State*	Princeton*
		Kentucky	Wyoming
		Wyoming	Kentucky
3	Advanced Combustion	Texas A&M*	Princeton*
	Carbon Storage	Penn State	LSU
		MIT	Pittsburgh
	Carbon Use & Reuse	Wyoming	Penn State
	Rare Earth Elements	Kentucky	Penn State

*Projects were selected for funding

UNIVERSITY COLLABORATION IN PROPOSALS CONT.

Solicitation Round	Topic Area	Lead University	Subcontracting University
4	Coal Beneficiation	Penn State	Utah
		West Virginia	Virginia Tech
		West Virginia	Virginia Tech
		West Virginia	Virginia Tech
5	Carbon Capture	Wyoming	Princeton
		Penn State	Wyoming
		West Virginia	Kentucky
	Gasification Systems and Coal Biomass to Liquids	LSU	Wyoming
6	Crosscutting Research	Penn State	Ohio State
	Carbon Capture	Penn State	Wyoming
		Wyoming*	Penn State*

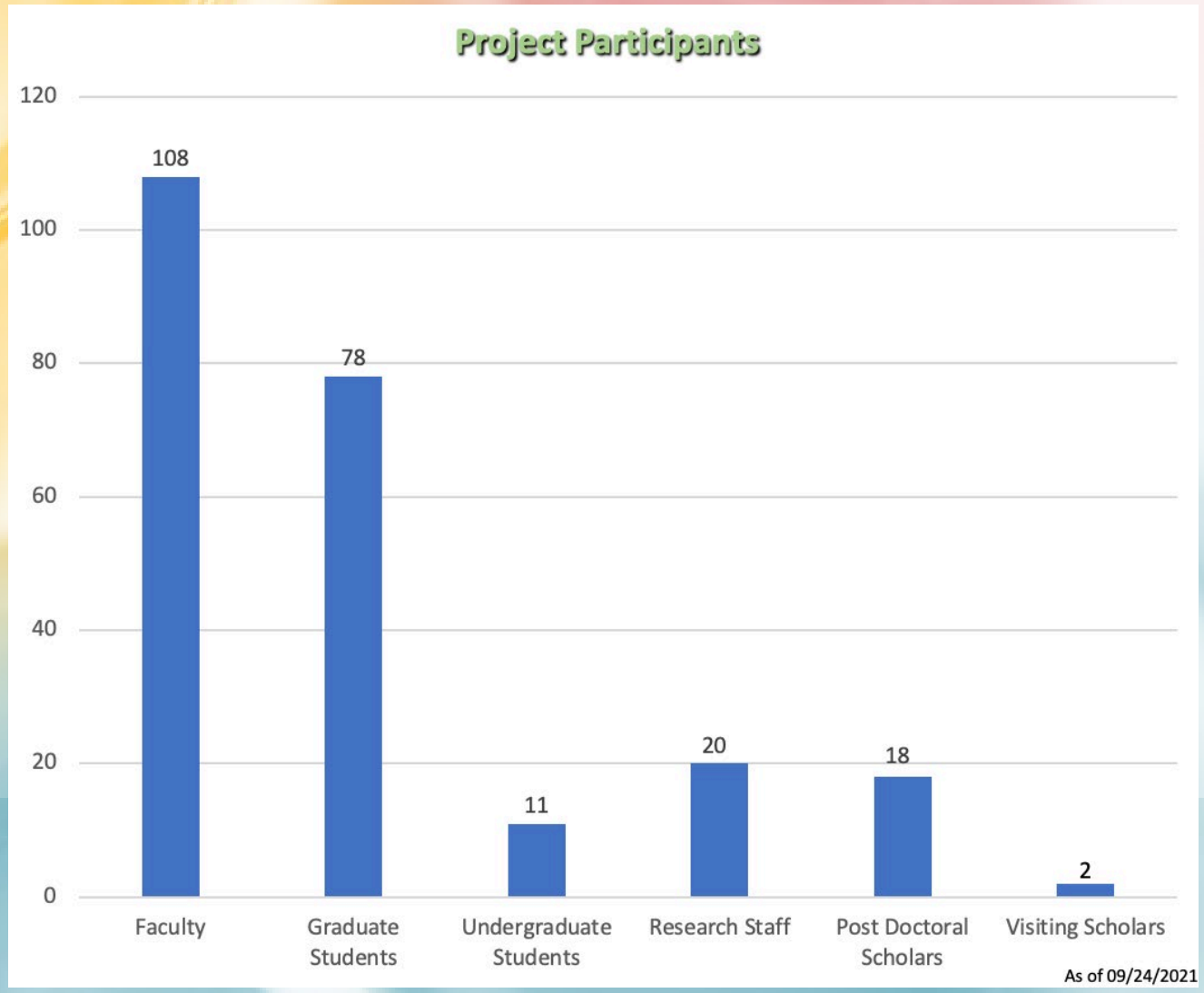
*Projects were selected for funding

COLLABORATION WITH NETL

- Collaboration between NETL and the individual projects is a major requirement for all funded projects. Examples of collaborative efforts are:
  - NETL staff time to support collaboration, consultation, technical guidance, sample analysis, and sample preparation
  - Internships at NETL
  - On-site testing and equipment usage by Coalition participants at NETL
  - Co-mentoring students
  - Co-authoring journal articles and conference papers

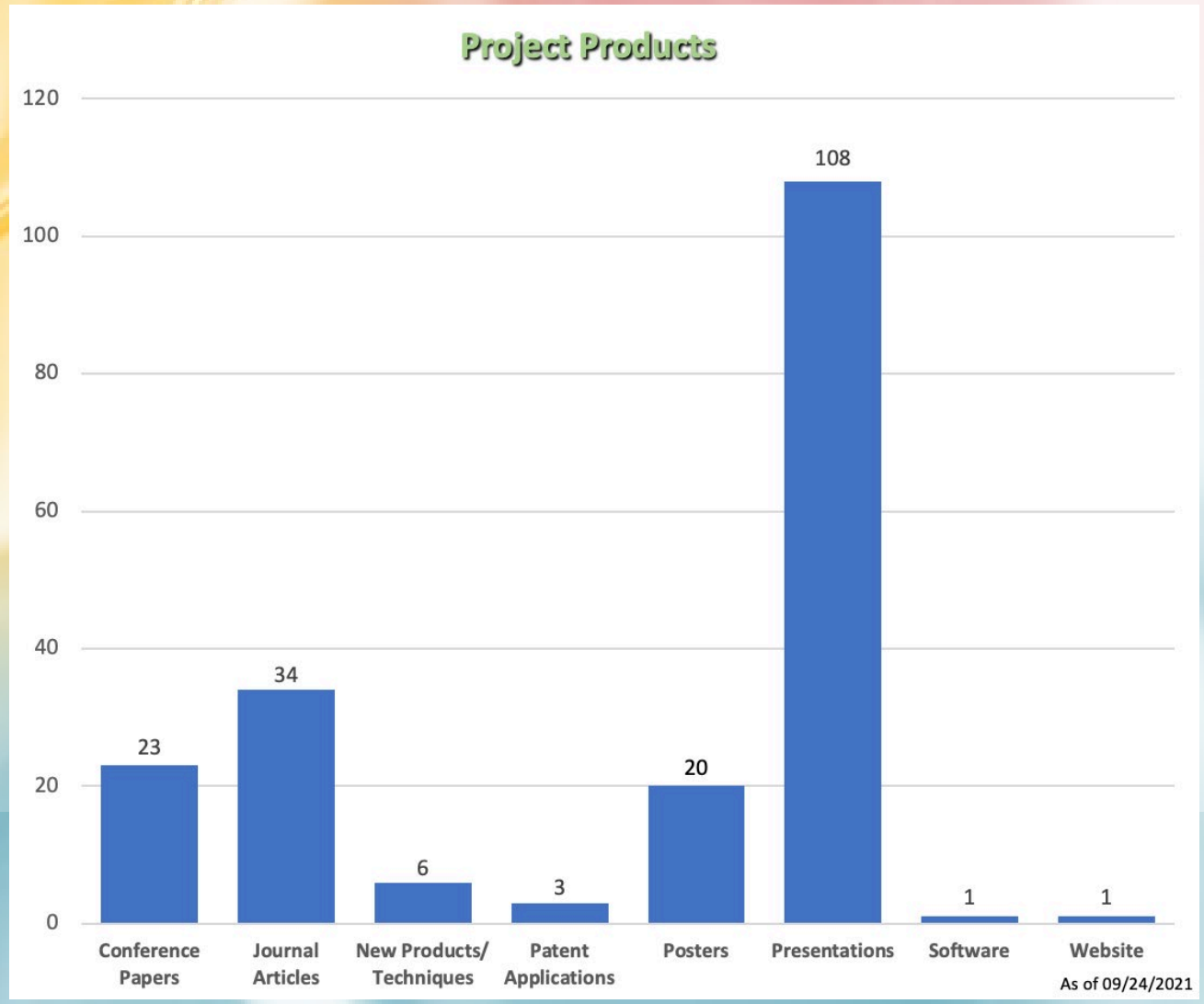
IMPACT OF UCFER PROGRAM

- Established the first national university alliance in fossil energy research with a major collaboration effort with DOE NETL that addresses specific topics in NETL's R&D mission areas.
- 237 participants (as of 09/24/2021)
- Generated inter-university collaborations:
  - 22 proposals contained collaborations out of 259 proposals submitted; ≈8%
  - 3 funded proposals contain collaborations out of 43 projects funded ≈7%



IMPACT OF UCFER PROGRAM CONT.

- UCFER projects have resulted in 10 cooperative research and development agreements (CRADAs) between NETL and universities that have been executed or are pending
- Non-coalition participants include 3 universities and 12 companies:
  - Subcontractor
  - Providing cost share (materials, analyses, cash)
  - Unpaid consultation and sample analyses
  - Advisory board members
  - Providing samples and materials for testing



OUTREACH ACTIVITIES

- UCFER website (sites.psu.edu/ucfer)
- UCFER session at the 45th International Technical Conference on Clean Energy- 'Clearwater' Conference
- Project summaries – prepared for completed projects with accepted final reports (16)
- Success stories – new activity; have reached out to PIs of completed projects

PURPOSE OF THE 'CLEARWATER' SESSION

- To provide an update of the NETL-PSU UCFER program (from the 2017 Clearwater conference)
- To showcase the range of projects and results
- Session started with an opening overview given by Penn State (Jennifer Matthews)
  - Summarizing the UCFER overview paper:
    - Overview of the NETL/Penn State Coalition for Fossil Energy Research Program authored by Bruce G. Miller, Jennifer Matthews, Elizabeth Wood (EMS Energy Institute) and Omer Bakshi and Madhava Syamlal (U.S. Department of Energy, National Energy Technology Laboratory)

PROJECT PRESENTATIONS

- Presentations were given on six projects after the UCFER program overview:
  - Penn State; S. Pisupati PI; topic area – Advanced Combustion
  - Louisiana State University; J. Spivey PI; topic area – Carbon Use & Reuse
  - West Virginia University; T. Musho PI; topic area – Gasification
  - Penn State; R. Vander Wal PI; topic area – Fuel Cell Technologies
  - University of North Dakota; X. Hou PI; topic area – Coal Beneficiation
  - Virginia Tech; C. Chen PI; topic area – Carbon Storage

EXAMPLE OF A PROJECT SUMMARY

Project Contact:
Ahmed F. Ghoniem
Ghoniem@mit.edu
(617) 253-2295

Project Lead Organization:
Massachusetts Institute of Technology

Other Participant:
Akhilesh Bakshi-MIT

Project Description:
The researchers developed frameworks for multivariate sensitivity analysis and uncertainty quantification as well as machine learning integration in Computational Fluid Dynamics (CFD) simulations.

1. Multivariate sensitivity analysis and uncertainty quantification: The team conducted multivariate sensitivity analysis using thirteen model input parameters and three dimensional (3D) CFD-DEM simulations with almost 170,000 glass bead particles (0.4 mm diameter) for a small-scale rectangular pulsating fluidized bed. Next, they investigated particle dynamics inside and around bubbles to derive an optimal criterion for the selection of normal spring stiffness as well as identified dilute areas in the bed as an ideal data set for the validation of the tangential damping coefficient.

2. Machine learning integration in CFD simulations: The team used a combination of physical insights and machine learning techniques to build a deep convolution network capable of mimicking the underlying dynamics of gas-solid multiphase flows.

Project Funding:
$134,000

Project Duration:
10/01/2016 -03/31/2018

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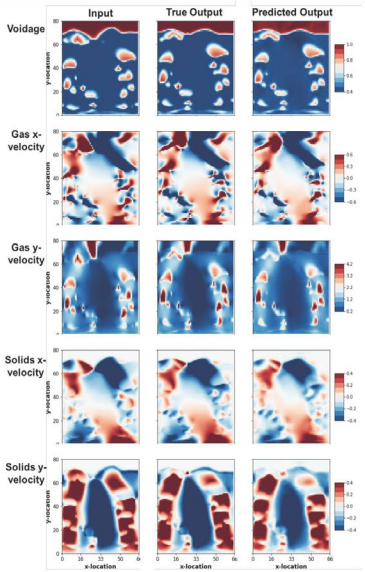
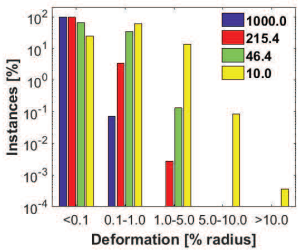
Grid Independence and Uncertainty Quantifications in Gas-Solid Flow Simulations

The major goals of this research were to develop tools for robust statistical analysis of multiphase flow simulations and integrate with NETL's MFiX suite; investigate the formation of patterns in pulsating gas-solid fluidized beds through high fidelity numerical simulations; develop a framework for integrating deep convolution neural networks with multiphase flow Computational Fluid Dynamics (CFD) towards more efficient simulations.



Benefits:
This work on multivariate sensitivity analysis was the first of its kind and establishes a robust framework for the statistical analysis of complex, highly-coupled simulations. By applying the developed methodology to CFD-DEM simulations, the scientists identified critical simulation parameters,established their coupled impact on dissipation dynamics,and proposed key guidelines for their selection.

Additionally, they demonstrated that deep convolution neural networks can successfully capture the underlying dynamics in computational fluid dynamic simulations. Although further study is required to optimize the network architecture and learning process, the established framework and developed tools will be extremely valuable for the simulation community.



August 2020

Accomplishments:
In this project, the scientists conducted an extensive multivariate sensitivity analysis, using MOAT approach, to determine the impact of model parameters on the accuracy of 3D CFD-DEM methods. Moreover, they used a combination of physical insights and ML techniques to build a deep convolution network capable of mimicking the underlying dynamics of multiphase flows, hence by accelerating CFD simulations.

Their results show that a smaller subset of the model parameters has a stronger impact on the predictions, including normal spring stiffness, normal restitution, inter particle and particle wall friction. Low normal spring stiffness, while popularly used for reducing the computational time, leads to unphysical and highly compacted dense phase by affected the particle velocities. Moreover, the impact of contact dissipation parameters is tightly coupled and sensitivity to any one parameter hinges on the choices of others. They showed that the choice of these parameters impacts the predicted stability of bubble patterns, where nearly elastic collisions and strongly dissipative dynamics lead to inaccurate prediction.

The ML model (deep convolution network) was developed using regression and feature scaling, while splitting available data between training, validation,and test data. The model was shown to make excellent predictions for bubbling fluidization and can be easily generalized to other operating conditions by training on diverse data sets and/or dynamic, and in situ optimization for re-tuning network weights.

NETL Collaboration:
The team collaborated extensively with the Validation, Verification and Uncertainty Quantification (VVUQ) team at NETL through bi-weekly teleconferences and group discussions on technical aspects of the statistical analysis and modeling approach; exchange of simulation and post-processing tools; and documentation of updates, including manuscripts for peer-reviewed journals and conference presentations.

Relevant Publications:
Bakshi, A., Li, T., Altantzis, C., Rogers, W., Shahnam, M, and Ghoniem, A.F., Comprehensive multivariate sensitivity analysis of CFD-DEM simulations: critical model parameters and their impact of fluidization hydrodynamics, Power Technology, 2018, 338, 519-537.

Bakshi, A., Altantzis, C., Bershanska, A., Stark, A., and Ghoniem, A.F., On the limitations of 2D CFD for thin rectangular fluidized bed simulations, Powder Tech. 332 (2018) pp. 727-637.

Software code for machine learning integration with CFD: https://github.com/akhileshbakshi/ConvNet.

www.energy.psu.edu/ucfer

SUCCESS STORIES

- Examples of information requested from PIs of completed projects (not inclusive):
  - New projects that have been funded as a result of UCFER funding
  - New commercial products
  - Establishment of a new center
  - New patent
  - New software
  - Best paper awards
  - Highly-cited work
  - Graduate student successes

ACKNOWLEDGEMENTS

- NETL leadership, technology managers, core competency leaders, project managers, and NETL's team working with UCFER on a regular basis
- Technical Advisory Council and Core Competency Advisory Board representatives, Executive Council members (past and current), and faculty participants and leaders of the 15 member universities
- All UCFER research participants at member universities and at NETL
- Penn State leadership supporting UCFER
- UCFER's Operations Management Team and others at Penn State