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Final Technical Report

Energy Frontier Research Center (EFRC): Center for Mechanistic Control of Unconventional Formations (CMC-UF)
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3. Executive Summary

The overarching mission of the Center for Mechanistic Control of Unconventional Formations (CMC-UF) was to garner cross-cutting, fundamental, geoscience knowledge to achieve mechanistic control over the strongly coupled nonequilibrium physical and geochemical processes in extreme geological environments including shale, mudstone, marls, and other tight rocks with nanoscale pores. Collectively, these are referred to as unconventional formations and they often play the role of seals for other subsurface storage formations, see Fig. 1. The fundamental knowledge garnered by CMC-UF enables science-based management of US unconventional formations for subsurface storage of carbon dioxide and TWh quantities of renewable energy as hydrogen and/or compressed air over longer timeframes as well as for natural gas production, with reduced environmental impacts, in the short term

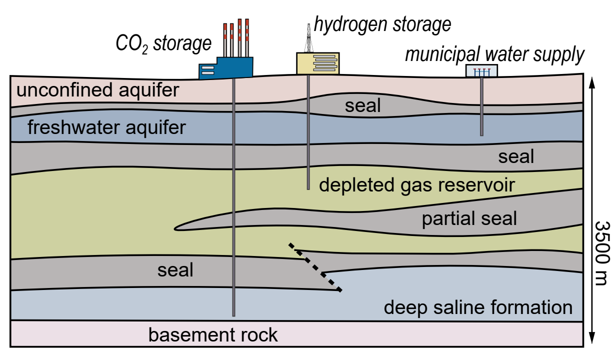


Fig. 1. Typical geological strata with seals (unconventional formations). Gas reservoir is repurposed for seasonal H_2 storage. The reservoir seal prevents vertical H_2 movement. Anthropogenic CO_2 is injected into a deep saline formation for secure storage. Top and bottom seals confine CO_2 to the formation.

CMC-UF team members acquired comprehensive fundamental experimental knowledge of geological seals and developed predictive models of the coupled physical, mechanical, and chemical processes that govern mass transport, deformation, reactivity, and storage within their multiscale pore space. In short, CMC-UF members wove a synergistic braid of experiments, theory, and computational modeling during the Center lifetime, 2018 to 2024.

Advanced multiscale and multimodal imaging as well as experimental characterization capabilities were exploited to analyze the textural fabric of disordered nanoporous media at nm to m scales before, during, and after interaction with aqueous and nonaqueous fluids (e.g., CO_2). These new experimental workflows and image analysis methods aided elucidation of the coupled phase behavior, geomechanical, and transport mechanisms of single and multiphase flow through nanoporous media across cascading length and time scales to understand, model, and control both conduits and barriers to transport. Delineation of reactivity at shale-mineral interfaces combined with fluid and solute transport revealed that shale surfaces are among the most reactive in the subsurface due to substantial compositional heterogeneity and large surface area of reactive surfaces. **Knowledge of the interplay of water composition, fluid flow conduits, stress**

with rock matrix composition and microfracture topology enables control through geochemical processes that can be engineered to either open pore space to flow or, conversely, close fractures and other pathways for rapid flow and thereby reduce transport through seals. The CMC-UF team characterized mechanisms of fracture closure under the influence of stress and reaction as well as the mechanisms of viscoplasticity and ductility of shale barriers when exposed to brine that are all important in determining the durability of reservoir seals. Throughout the scientific effort, integration and translation of physical and chemical mechanisms was accomplished using advanced algorithms and modeling to assess the influence of fine-scale processes at macroscopic length and time scales.

Notable advances are summarized as follows.

- We developed new workflows to collect and integrate characterization data from multiple instruments to solve the scientific puzzle of pore structure and connectivity of multiscale nanoporous geomaterials.
- We decoded the coupled nonlinear behavior of complex systems using both bottom-up and top-down models, combined with multiscale characterization data where it was impractical, or impossible, to create experimental conditions with outcomes that were measurable directly.
- We measured and modeled chemical reactions to understand how the many interfacial processes in heterogeneous solid-liquid and solid-gas phase systems control dissolution, adsorption, deposition, and mechanical failure.
- We built robust predictive models of highly complex, multiphase, heterogeneous, and reactive natural systems incorporating holistic spatiotemporal scale integration.

4. Science Questions

The research approach within CMC-UF was guided by 11 cross-cutting science questions that required a multidisciplinary approach to answer. These questions were the north star guiding CMC-UF efforts toward science-based management of the US shale resource for reduced environmental impacts of natural gas production in the short term and, importantly, foundational understanding for building subsurface hydrogen and carbon dioxide storage infrastructure as well as geothermal energy recovery. A description of the 11 CMC-UF specific science questions follows:

1. How are shale compositional and structural heterogeneities, interfaces, and disorder characterized and how do these attributes control the behavior & performance within this natural energy system?
2. How are characterization data from multiple sources integrated and extended to solve the scientific puzzle of multiscale, multiphysics processes in multiscale porous media?
3. How do complex fluids wet the heterogeneous surfaces of natural porous media, i.e., shale?
4. How does sorption interplay with transport to determine permeability and mechanical properties?
5. How do the many interfacial processes in heterogeneous solid-liquid and solid-gas phase systems control dissolution, adsorption, deposition, and failure?

6. How do we achieve mechanistic control of interfaces and transport in extreme environments?
7. How are experimental and simulation data transformed into practical information?
8. How is a predictive understanding of subsurface system behavior developed that embraces multi-scale complexity, dynamics, and reactivity across approximately ten orders of magnitude length. scale?
9. How are robust predictive models developed for highly complex, multiphase, heterogeneous, and reactive natural systems?
10. How are numerical algorithms advanced to reach across traditional mathematical boundaries to generate computer models of sophisticated, coupled, multiscale phenomena and experiments to understand data?
11. How are theory, computation, and experiment combined to probe the structure, chemistry, mechanics, and response of complex natural systems?

The efforts to answer these questions propelled the CMC-UF team to garner significant fundamental knowledge and to develop comprehensive models of coupled, multiscale processes. Meeting these science goals provided fundamental understanding of chemical transformation and transport in nonequilibrium, heterogeneous, nanoscale environments. Our research probed the geochemical and geophysical processes at the fine scale to understand mineral/fluid interactions and chemical transport and pushed the boundaries of current measurement methods and data science approaches to integrate experimental results, models, and data.

5. Accomplishments

The CMC-UF approach was multidisciplinary geoscience and was summarized in our reviews of scale translation and reactivity of unconventional formations (Mehmani et al. 2021, Khan et al. 2021, Jew et al. 2022). We pioneered innovative workflows for spatiotemporal scaling with the potential to overcome the fundamental lack of scale separation in unconventional rocks (Liu et al. 2024). We discovered and documented that the mineral/fluid interface in these systems is among the most reactive in the subsurface (Khan et al. 2021, Nöel et al. 2023, Murugesu et al. 2024a). We developed and exploited imaging and image reconstruction modalities with nm resolution to understand shale fine-scale rock fabric (Frouté and Kovscek 2020, Frouté et al. 2023) and performed transport calculations on such images (Anderson et al. 2020b, Frouté et al. 2020, Liu et al. 2024). These advances provided the basis of CMC-UF's accomplishments in our mission to unravel and control the interplay of heterogeneity, fluid/mineral reactivity, and stress.

The remainder of section 5 summarizes the findings of the CMC-UF team in response to the 11 science questions asked above.

5.1 How are shale compositional and structural heterogeneities, interfaces, and disorder characterized and how do these attributes control the behavior & performance within this natural energy system?

We observed shale fabric, mineralogy, and porosity and integrated observations with numerical simulations to reveal the physical mechanisms limiting transport at various scales. No single experimental or numerical approach completely characterizes the complexity of shale reservoirs at all scales (Mehmani et al. 2021). To meet this challenge, we integrated experimental techniques from across CMC-UF in novel ways, including electron, X-ray, and optical microscopy, as well as nuclear magnetic resonance, positron emission tomography, and X-ray absorption spectroscopy (Anderson et al. 2020a,b, Ling et al. 2022, Nöel et al. 2023, Zahasky et al. 2023). The sum of these techniques paints a complete picture of the physical and chemical properties of shale from the centimeter to nanometer scale. In order to integrate observations across scale, we developed novel methods for image registration and data assimilation (Anderson et al. 2021). All the samples used in our experimental studies were from a single shale formation, where we used well logs, microseismic monitoring, and borehole stress measurements to model production, slip on existing fractures (Alshafloot et al. 2024), and hydraulic fracture propagation (Alshafloot et al. 2024, Yang et al. 2021 & 2023). By placing our experimental samples in the context of field data, we connect our observations of fundamental physics to operational parameters and efficiency metrics.

5.2 How are characterization data from multiple sources integrated and extended to solve the scientific puzzle of multiscale, multiphysics processes in multiscale porous media?

We developed and adapted machine learning and statistical techniques to integrate, extend, and translate diverse multimodal and multiscale data of porous media into meaningful applications and representations for understanding multiscale and multiphysics phenomena. Our efforts have focused on data translation between imaging modalities as shown in Fig. 2, image downscaling in the form of image super-resolution, and data synthesis for porous media images (Anderson et al. 2020a, Anderson et al 2021, Ling et al. 2021, Murugesu et al. 2024b). Each of these efforts extends our characterization capabilities and thereby furthers our understanding of multiscale/multiphysics porous media. Data translation models allow us to predict high-contrast nanoscale images and image volumes from low-contrast/low-resolution nondestructive input data (Anderson et al. 2020a). These algorithms preserve samples for further experimentation while providing image data with comparable resolution and contrast to destructive imaging modalities. Image downscaling, meanwhile, allows us to predict low-throughput/high-resolution images from high-throughput/low-resolution data (Murugesu et al 2024a). Such an imaging setup enables dynamic imaging of reactive transport processes at both sufficient time and spatial resolution to understand the system dynamics. Finally, data generation allows us to extend limited, costly, or destructive image data of shale fabric and microfracture networks by building models to sample statistically synthetic images of samples and to use these to quantify uncertainty in petrophysical properties (Anderson et al. 2021). Beyond image processing, generation, and analysis, the data representations learned by these multiscale/multimodal image assimilation models are applied to modeling and analyzing multiphysics/multiscale physical and chemical processes (Wang and Battiato 2021).

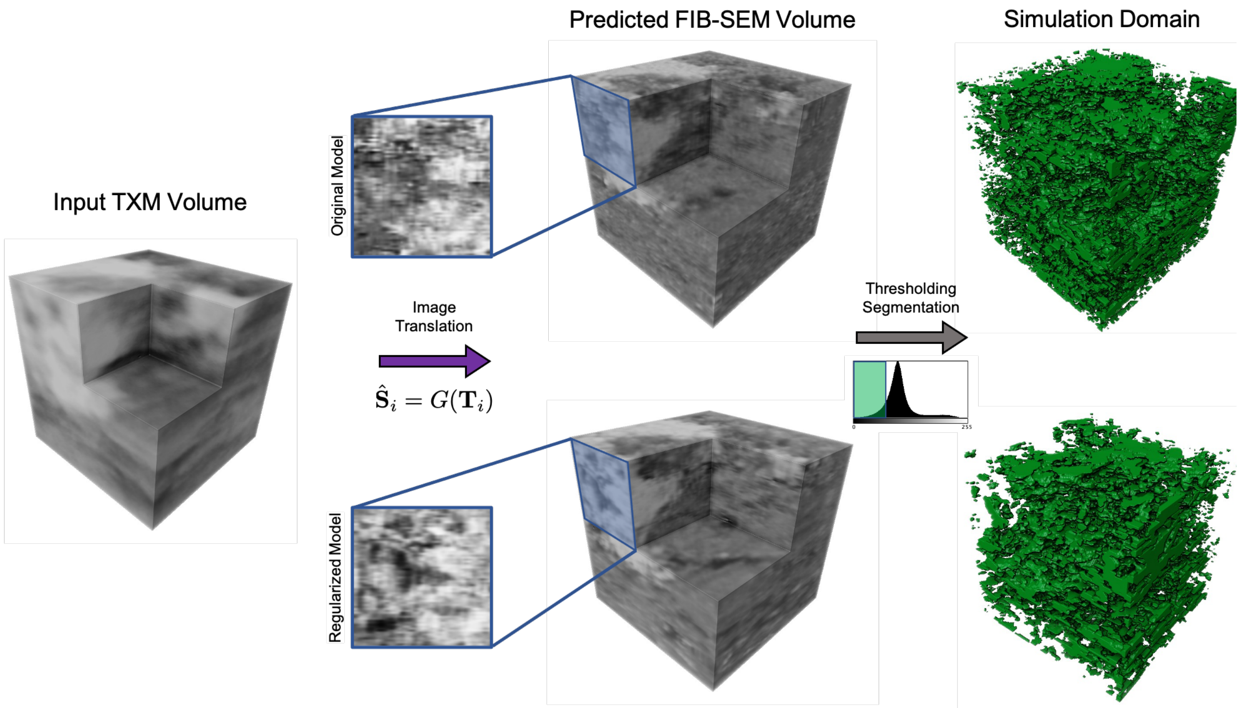


Fig. 2. Example of multimodal image translation and generation of domain for transport simulation (Anderson et al. 2021). On the left is an input transmission x-ray microscope (TXM) image of a shale volume. TXM is nondestructive. Machine learning is used for image translation to predict an image of a high-contrast scanning electron microscope (FIB SEM) reconstruction of the pore space. FIB SEM is a destructive imaging technique. After segmentation of the FIB SEM volume, an image of pore space is obtained on the far right.

5.3 How do complex fluids wet the heterogeneous surfaces of natural porous media, i.e., shale?

We used a multipronged approach that cross-cut length scales and entails experiments as well as theory to address the fundamental question of gas, water, and organic phase wetting of heterogeneous surfaces. Characterization of the shale fabric and nanopore structure provides the basis for diverse integrated studies of wetting including molecular dynamics of water and carbon dioxide in nanopores and microcracks, upscaling using Minkowski functionals (Simeski et al. 2020, Boelens and Tchelepi 2021a), nuclear magnetic resonance spectra as shown in Fig. 3 (Medina-Rodriguez 2021), measurement of the microscopic details of reaction product evolution in microfluidic devices (Ling et al. 2022), direct numerical simulations incorporating wetting and phase behavior, and adsorption (Esmeailzadeh et al., 2020, Boelens and Tchelepi 2021b). We find that fluids wet heterogeneous surfaces in surprising ways with results depending upon pressure, temperature, reaction rates, phase composition, and the mutual solubility of chemical components in different phases. Condensation within nanopores is an important manifestation of wetting that is being understood within the experimental-theoretical-upscaling framework described above (Rehmeier et al. 2023, Simeski et al. 2023). Importantly, stronger electrostatic moments, all other factors equal, lead to greater adsorption and condensation at low pressures (Simeski et al. 2020).

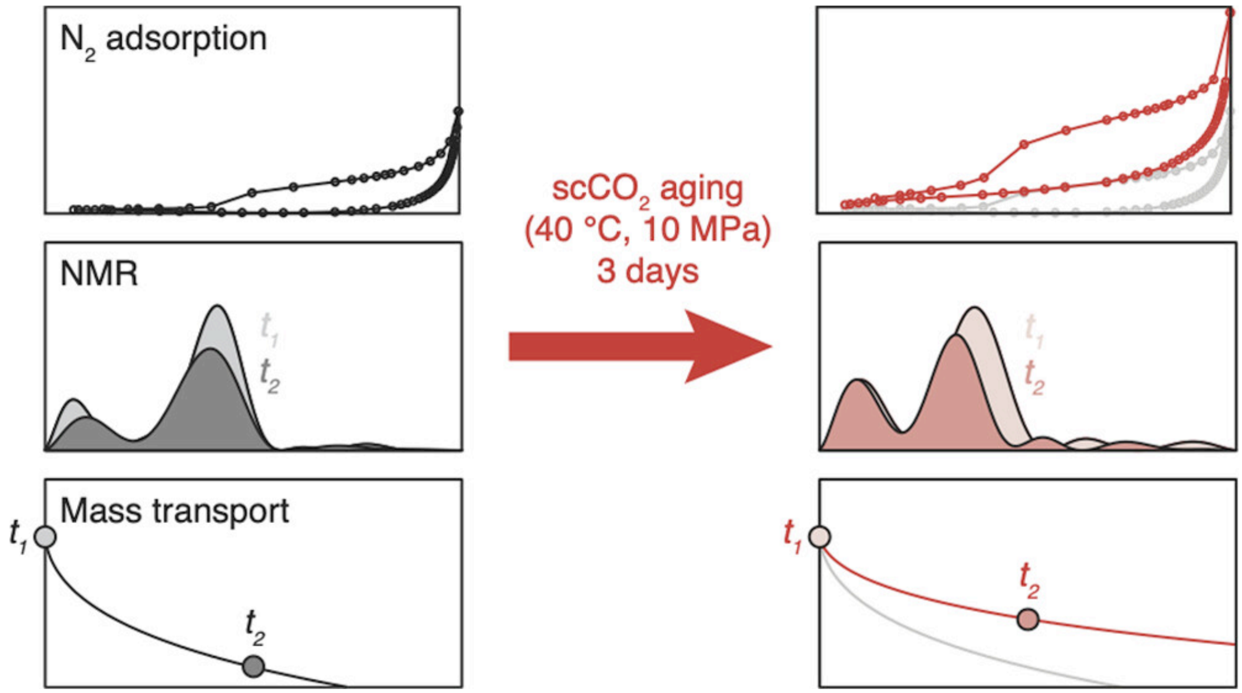


Fig. 3. Characterization of shale pore sizes and structures before and after exposure to $scCO_2$ using a combination of gas adsorption and nuclear magnetic resonance (Medina et al. 2023). Integrating the gas adsorption and NMR data shows how supercritical CO_2 injection alters the pore-size distribution for pore sizes <1 nm to 1 mm. Results provide insights on how the pore structure and mass transport properties of different shale lithologies may evolve during storage of supercritical CO_2.

5.4 How does sorption interplay with transport to determine permeability and mechanical properties? **We unraveled the fundamental details of coupled sorption, transport, and mechanics across length scales with coordinated experiments, modeling, and upscaling.** CMC-UF researchers endeavored to work on identical or similar samples providing substantial leveraging of measurements and the provision of data for model development and calibration. The pulse decay method (i.e., gas expansion) of interrogating the transport properties of tight media measures flow dynamics of CO_2 in shale under reactive conditions (Lyu et al. 2021), displacement of resident gases such as methane, and the interplay of transport and adsorption all under conditions of stress. X-ray computed tomography of the dynamics of CO_2 movement relates macroscopic location and distribution of CO_2 to microscopic details of shale fabric (Elkady et al. 2020). Overarching results indicate that moist shales containing carbonate minerals are reactive in the presence of CO_2 and subject to mechanical weakening (Kamali-Asl et al. 2021 & 2022). Dual continuum models (i.e., those that consider the fracture network and shale matrix as separate interacting continua) effectively represent the dynamics and adsorption of gases in mesoporous and microporous segments of shale within an upscaled model as shown in Fig. 4 (Lyu et al. 2021, Lyu et al. 2023).

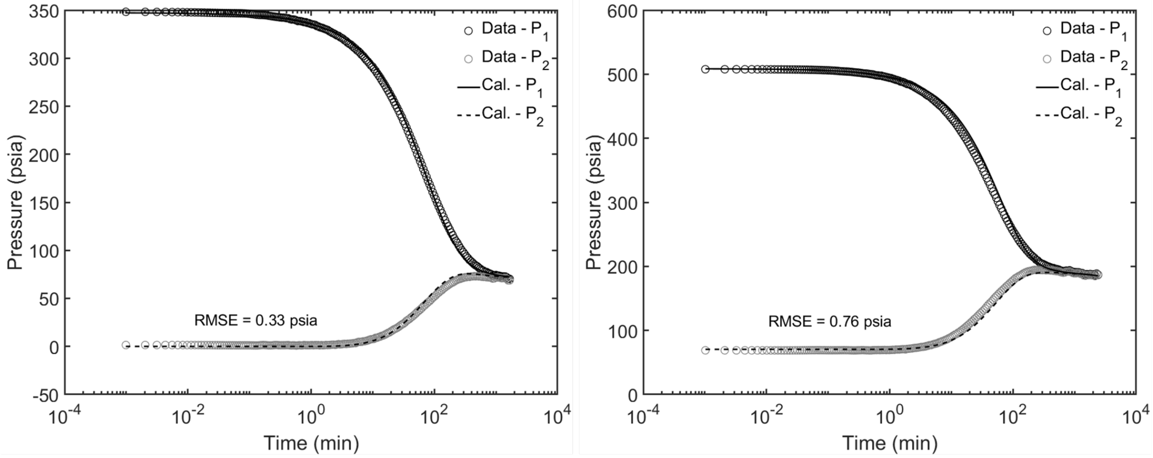


Fig. 4. Pressure pulse decay experiments (points) and dual porosity model predictions (lines) for a CO_2-shale system (Lyu et al. 2023). Results from separate low- and high-pressure experiments shown. The shale sample consists of natural fractures, microcracks, mesopores, and micropores. A modified analytical approach is used to evaluate the mass transfer rate in microcracks and mesopores. A triple-porosity model is then utilized to estimate the remaining parameters: the effective gas permeability in the fracture, the mass transfer rates in micropores, and the volume split between mesopores and micropores. Adsorption of CO_2 is included.

5.5 How do the many interfacial processes in heterogeneous solid-liquid and solid-gas phase systems control dissolution, adsorption, deposition, and failure?

The CMC-UF team measured and modeled chemical reactions at mineral/organic matter/hydraulic fracture fluid (HFF) interfaces because they play major roles in the extraction of hydrocarbons from unconventional oil/gas shales as well as control the long-term performance of seals overlying carbon dioxide storage formations. We find that interfaces in shales are exceptional microenvironments governed by far-from-equilibrium reactive conditions (Khan et al. 2021, Jew et al. 2022). The pH of fluids delivered to these interfaces may be negative on the log scale and such fluids may spontaneously imbibe into unsaturated shale at rates of as high as 10 mm/s across a narrow depth into the shale interior (Nöel et al. 2023). At these acidities and velocities, reactive alteration creates measurable changes to shale flow and mechanical properties. Reactions of acidic fluid with inorganic and organic phases in unconventional shales result in (1) dissolution of mineral phases such as pyrite (FeS_2), calcite ($CaCO_3$), and barite ($BaSO_4$) (from drilling muds), which releases Fe^{2+}, Ca^{2+}, and Ba^{2+} cations (and trace amounts of heavy metals) and increases porosity and permeability, particularly in carbonate-rich shales; (2) oxidation of aqueous Fe^{2+} to Fe^{3+} and of aqueous S^{2-} to SO_4^{2-}; and (3) (re)precipitation of Fe^{3+}-(oxyhydr)oxide, calcite, barite, strontianite ($SrCO_3$), and celestite ($SrSO_4$) in the fracture network, that reduces pore connectivity and permeability (Medina 2022, Medina-Rodriguez et al. 2023). Mineral solubilization increases permeability and may lead to matrix weakening while attendant mineral precipitation and sorption decrease permeability and impede fluid penetration. The competition among dissolution and precipitation mechanisms ultimately determines the transport and mechanical properties (Kamali-Asl et al. 2021, Murugesu et al 2023). These reactions also impact the release and sequestration of trace levels of heavy metal contaminants (Cr, Ni, Cu, Zn, Se, and U) that are common in many organic-rich black shales (Jew et al. 2020).

A major component of our study was reactive transport modeling of these processes, with the aim of developing a new model of reactive imbibition that allows us to examine the major variables controlling element transport during hydraulic fracturing of unconventional shales in a quantitative, predictive fashion. At the core scale, we tracked the impact of interface alterations using coordinated tests for permeability before, during, and after exposure to nonequilibrated fluids such as brine saturated with supercritical CO_2. We created the protocols necessary for shale embedded microfluidics, see Fig. 5, demonstrating the utility of this important emerging methodology to monitor the reaction progression and irreversible changes to shale fabric under flow conditions at resolutions appropriate to detail the fluid-shale interface (Ling et al. 2021, Ling et al. 2022). Importantly, we used microfluidics to understand achievement of mechanistic control, as described next.

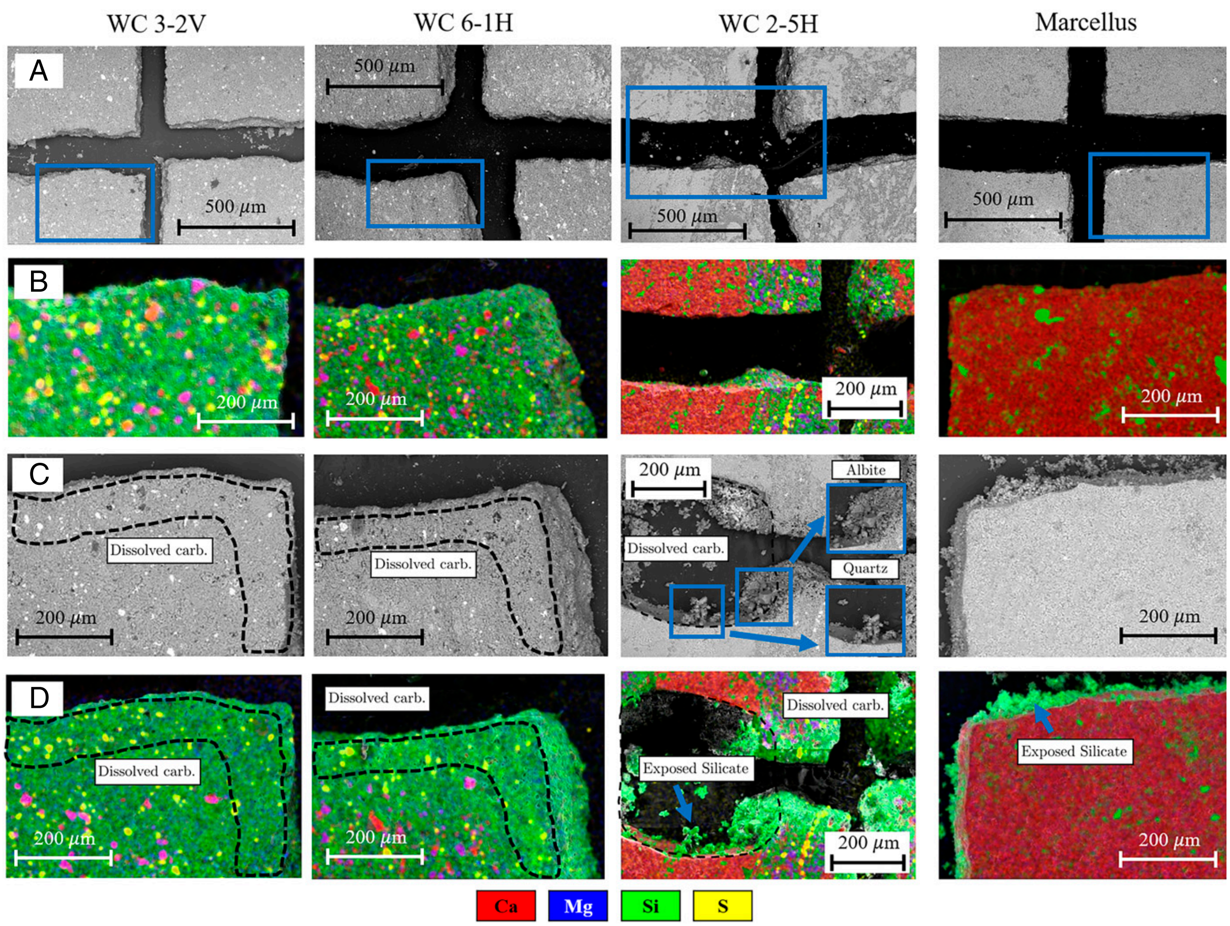


Fig. 5. Results from a shale-embedded microfluidics device that was designed to probe and quantify interfacial processes (Ling et al. 2022). (A) Prereaction scanning electron microscope backscattered electron (SEM-BSE) images of the four samples (image width = 1.38 mm). Blue boxes (image width ~0.5 mm) correspond to select regions prereaction and postreaction images in B–D. (B) Prereaction composite elemental maps for the select region. (C) Postreaction SEM-BSE images of the same region. Insets show albite and quartz crystals exposed after the dissolution of surrounding calcite. (D) Corresponding postreaction composite elemental maps. Samples are ordered from carbonate-poor on the left to carbonate-rich on the right. The interfacial dissolution zones with newly developed porosity are indicated by dashed lines. The dashed region for WC 2-5H corresponds to calcite dissolved from both sides of the fracture. The colors indicate individual elements as listed for each composite element image.

5.6 How do we achieve mechanistic control of interfaces and transport in extreme environments?

We developed and used models to assimilate experimental and theoretical knowledge about both flow and the chemical reactivity processes that either enhance or decrease permeability in shales. Deep subsurface energy systems rely upon controlled stimulation of host rock using hydraulic fluids to enable exchange of heat, CO_2, or hydrocarbons. In the process, injection of fluids initiates a tapestry of fluid-rock reactions, that inevitably leads to dissolution and subsequent mineral scale precipitation, mechanical weakening of fracture faces, and ultimately, closure of pore throats and fractures (Ling et al. 2022, Murugesu et al. 2023). Reactive transport models (RTMs) are increasingly important for developing mechanistic controls of interfacial chemistry and transport in shales (Nöel et al. 2023). To provide experimental data needed to build next-generation flow and RT models, we made experimental observations across scales, from nano- to millimeters through a series of interlinked collaborative activities. CMC-UF team members published three interconnected papers that advance fundamental understanding of this reactive transport in shales: (a) We used Scanning Electron Microscopy (SEM), Focused Ion Beam Scanning Electron microscopy (FIB-SEM) and Scanning Transmission Electron Microscopy (STEM) to perform a correlative cross-scale study of porosity and pore connectivity (Froute *et al*, 2020). (b) This information then informed the development of the first microfluidic model to span from Darcy to pore scales as shown in Fig. 5, (1 µm to 100 mm) (Ling *et al*, 2021). This direct-observation flow system was instrumental to explore the combined impacts of scaling behavior and network geometry on fluid transport. (3) To further understand and model the coupling between fast flow events such as imbibition and chemistry, we used synchrotron X-ray fluorescence mapping to directly and simultaneously image fluid transport and evolving chemical reaction fronts at the microfracture scale as shown in Fig. 6 (micrometers to centimeters) (Noël *et al*., 2023). Assimilation of processes and data observed in these studies is currently driving a rapid expansion of model simulation capabilities and transformed our ability to control mechanistically shale interfaces.

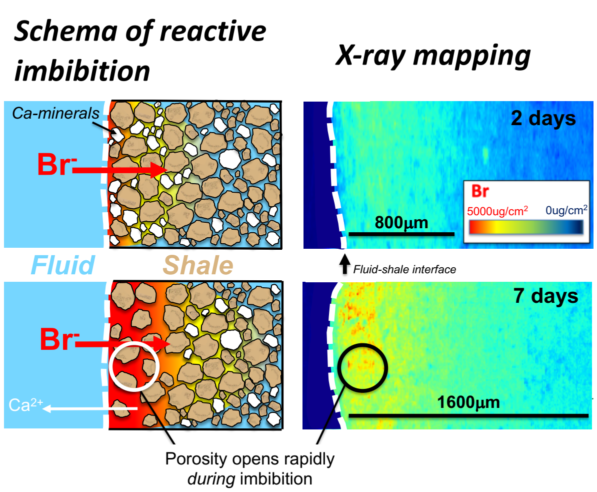


Fig. 6. Schematic representation (left) and x-ray imaging of bromide tracers (right) reveals a previously unknown type of reactive transport in shale, termed "reactive imbibition" (Nöel et al. 2023). Calcite dissolution is triggered and proceeds at roughly the same rate as rapid spontaneous imbibition of acidic stimulation fluids, allowing the two processes to interact in unexpected ways, and causing penetration of fluids to be dependent on evolving porosity changes.

5.7 How are experimental and simulation data transformed into information?

Scientific discovery involves the formulation of theory to explain observed experimental data and, importantly, the design and execution of experiments to test and evolve theory. Transformation of data into useful information was achieved through integrating data interpretation, modeling constrained by experimental data, and machine learning (Wang and Battiato 2021, Anderson et al. 2021, Huang et al. 2022). Combining experimental and simulation (based on the theory) data provides crucial information to better constrain our understanding and prediction of fluid-solid interactions, transport fluid/gas inside rock (Wang and Aryana 2021, Liu et al. 2021), and mechanics. Dynamic and static imaging, spectroscopy, microscopy and relaxation time were among the most powerful data types for probing in situ processes that we pursued (Perez Claro et al. 2021). We incorporated the outcomes of such measurements into at-scale computations using density functional theory, molecular dynamics, lattice Boltzmann method, direct numerical simulation, micromechanical, and other continuum scale techniques to probe fundamental physical processes. In many cases, we use both multiscale data and models to translate between length scales using formal upscaling/downscaling, Minkowski functionals, and machine learning techniques.

5.8 How is a predictive understanding of subsurface system behavior developed that embraces multi-scale complexity, dynamics, and reactivity across approximately ten orders of magnitude length scale?

Our approach was holistic and was characterized by comprehension that at-scale shale features, physics, and chemistry are intimately coupled and that effects cascade across the length scales defining the system. This understanding was critical for appropriate model selection and development at larger scales, as well as for model parameter estimation, necessary to achieve predictive understanding (Lyu et al. 2023). Important physical and chemical features cascade across length scales and so does our research approach (Mehmani et al. 2021). Scale translation remains the ultimate challenge. Much of the physics and chemistry of shale-fluid interactions occurs within the nanoporous regions including sorption and reaction (Edgin et al. 2021, Medina-Rodriguez 2021, Medina-Rodriguez 2023), while the emergent behavior occurs over geological formations characterized by km-scale distances between wells. Intermediate length scales of the fractured domain are important for transport of acidic fluids and mixing with the resident brines. The critical question is how physics at the nanoscale are appropriately accounted for at the larger scale. Our model development effort was directly guided by the natural system. We used SEM/TEM/XAS/NMR as appropriate methods to help understand the smaller scales and the linkages among scales (Frouté et al. 2023, Medina-Rodriguez et al. 2023). The experimental techniques are complemented by molecular simulation methods such as MD, GCMC, DFT, and so on, supporting development of both computationally efficient and physically accurate models at larger scales. Lattice Boltzmann method simulations provide a link from the nanoporous to the pore network scale and, hence, continuum effects, thereby incorporating nanoporous dynamics at larger scales (Liu et al. 2024). The integrated result of nanoporous transport and reaction mechanisms was measured using micro and clinical tomography (CT and PET) coupled with time-resolved solute generation and reactive transport model development (Zahasky et al. 2019, Zahasky et al. 2023, Murugesu et al. 2024a). These approaches give insight into sorption and solubilization at larger scales, gas transport and displacement, matrix softening, and, importantly, transport through microcracks and fractures (Kurotori et al. 2023).

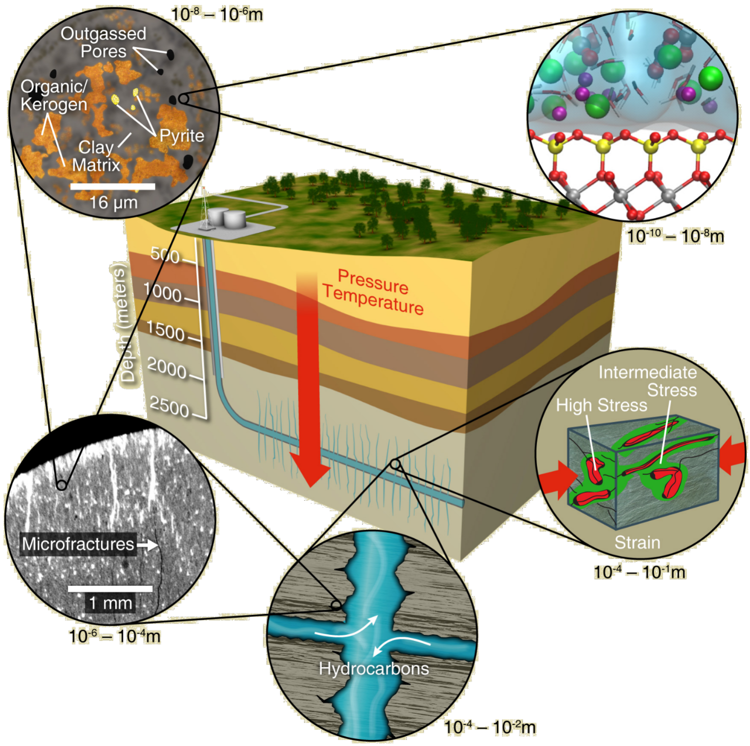
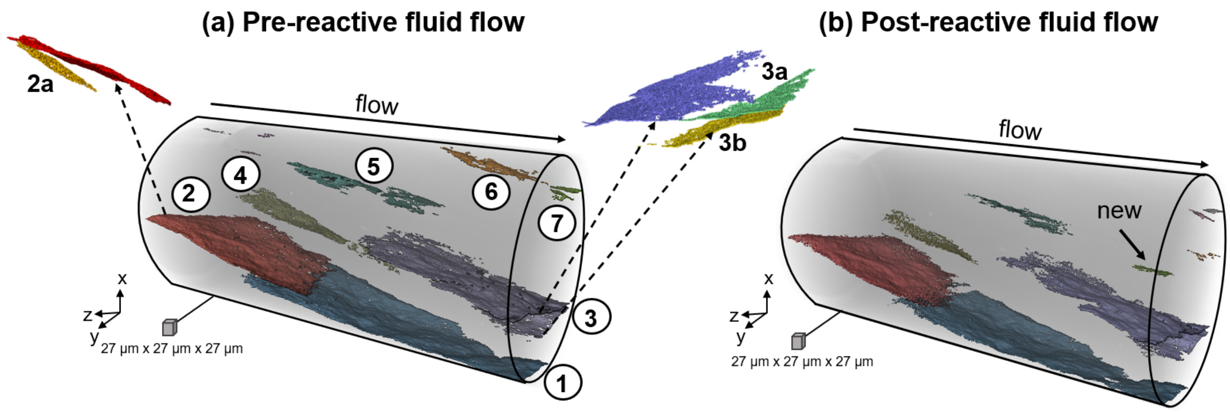


Fig. 6. Illustration of the cascade of length scales of interest in shale formations (Mehmani et al. 2021). From the upper right: water/clay interactions in a 10 nm wide slit pore where water is shaded in blue; nanoCT image of shale structure illustrating minerals, kerogen, and outgassed pores; microfractures filled with barite scale; matrix-to-fracture mass transfer; zones of enhanced ductility.

5.9 How are robust predictive models developed for highly complex, multiphase, heterogeneous, and reactive natural systems?

Our models were built from the bottom up as well as from the top down to decode the coupled behavior of complex nonlinear systems under conditions where it is impractical, or impossible, to create experimental conditions with outcomes that can be measured directly. Seal materials and shales are inherently multiscale with features cascading upward in length scale from pores to microcracks to fractures, Fig. 6. Fractures span from the scale of grain boundaries (nm) to formation boundaries (m) and may evolve in time as a result of mechanical or reactive processes. State of the art procedures for upscaling/downscaling, such as homogenization, fail due to lack of scale separation (Mehmani et al. 2021). Phenomena such as multiphase transport, phase behavior, geochemistry, and geomechanics, act in tandem and in complex patterns as illustrated in Fig. 7. The intricate interdependencies and feedback across scales, gives rise to macroscale behavior. We developed new algorithms to account properly for across-scale coupling when classical upscaled formulations are invalid, as is typical in reactive processes that involve precipitation and clogging (Wang and Battiato 2020 & 2021). We use robust models, informed by physical measurements, to untangle methodically the various mechanisms. We also use such models in predictive mode to integrate physics. The bases for combination across scales are image data, molecular dynamics, Minkowski functionals (geometric descriptors of porous media such as porosity, curvature, connectivity), and lattice Boltzmann simulations (Simeski et al. 2020, Boelens and Tchelepi 2021, Wang and Aryana 2019, Wang and Aryana 2021). Transport at microscale, and molecular interactions, is examined using atomistic scale simulation. Mesoscopic simulation techniques, such as the lattice Boltzmann method (LBM), are used as a means to link and translate the physics in fluids across scales by capturing the essential physics and tracking the collective behavior of the system (Frouté et al. 2020). This is done in computational domains that reflect the finely resolved characterization of pore spaces obtained using measurements from SEM and TEM (Liu et al. 2024). To date, we have expanded LBM to account accurately for complex geometries and confined phase behavior in nanopores. Phase behavior and transport are coupled in LBM via development of a confined extension of Peng Robinson cubic Equation of State (CEoS) and using this extension to inform intermolecular forces in confined systems in the LBM framework via a pseudopotential model (Wang and Aryana 2021, Liu et al. 2022). The LBM model is tuned and validated based on benchmark atomistic simulation data, and its use is extended to complex networks via the use of a preconditioner (Liu et al. 2021). Scalable implementations of LBM (Frouté et al. 2020, Rustamov et al. 2022) are then used to obtain input for continuum-scale models. The final picture emerging from examination of the interplay between different physical aspects, e.g., reactive transport and geomechanics, is that it is necessary to honor the full complexity of multiphase fluids within heterogeneous and reactive natural hierarchical permeable media.



Fracture	Length (mm)	Thickness (mm)	Width (mm)	Area (mm²)	Volume (mm³)
1	41.42	0.68	10.15	1295.02	53.44
2	29.94	0.59	5.48	928.81	38.49
2a	12.87	0.25	3.17	100.85	2.85
3	25.17	0.77	5.56	709.01	24.58
3a	17.97	0.44	4.99	183.65	5.85
3b	16.12	0.32	3.66	189.91	6.05
4	30.10	0.31	2.95	333.14	9.11
5	23.98	0.89	4.92	354.30	8.23
				Total Volume	148.60

Fracture	Length (mm)	Thickness (mm)	Width (mm)	Area (mm²)	Volume (mm³)
1	43.66	0.43	9.65	1190.22	32.12
2	27.31	0.53	3.42	897.28	23.81
2a	9.96	0.24	2.18	66.26	1.15
3	25.33	0.60	3.81	551.76	12.56
3a	14.44	0.18	2.65	154.85	3.78
3b	15.34	0.29	4.41	97.56	2.16
4	20.43	0.33	2.59	195.88	3.19
5	17.03	0.40	3.48	131.35	2.03
				Total Volume	80.80

Fig. 7. X-ray micro computed tomography images of a fractured shale core subjected to acidic reactive fluid under confining stress as an analogy to brine acidified with carbonic acid (Murugesu et al. 2024): (a) pre-reactive flow shows ample fractures identified and numbered and (b) post-reactive flow shows that fracture width, area, and volume decrease as a result of reactive transport processes under stress that closes fractures. Sample permeability decreased by a factor of 4 between images (a) and (b).

5.10 How are numerical algorithms advanced to reach across traditional mathematical boundaries to provide computer models of sophisticated, coupled, multiscale phenomena and experiments to understand the data?

We bridged boundaries through the development and application of machine learning methods. Image super-resolution models are integrated with experiments to enhance dynamic imaging of reactive transport processes at the fracture and macropore scale (Wang and Battiato 2021, Murugesu et al. 2024). This approach may be further integrated with simulation models to calibrate model parameters. In doing so, we provide a link across length and time scales between coarse-grid low-resolution image data acquired by experiment and fine-grid simulation data. Image data generation models allow for synthesis of image data across domains and scales (Anderson et al. 2021). Synthetic images are used in tandem with digital rock physics techniques to estimate and quantify uncertainty for morphological and petrophysical properties of samples when only limited or destructive imaging data are available. Furthermore, jointly synthesizing multimodal/multiscale data provides a link across data domains and scales that can then be correlated to simulated or experimentally observed transport properties in one of the domains or scales (Liu et al. 2024).

5.11 How are theory, computation, and experiment combined to probe the structure, chemistry, mechanics, and response of complex natural systems?

Imaging of nanopores in 3D provides a basis to probe coupled processes in complex nanoporous geological media. Experiments, theory, and computations have been combined to obtain fundamental understanding of transport, phase behavior, mechanics, and reaction within and outside nanopores as summarized in Fig. 8. Scanning transmission electron microscopy (STEM) provides superior resolution of the size, shape, and 3D connectivity of nanoporous networks (Frouté et al. 2023). Using such 3D pore network images, we have combined molecular dynamics with lattice Boltzmann method simulations to transform image data into information and to translate physics across length and time scales. For instance, direct estimation of nanoDarcy matrix permeability from image data has been obtained (Frouté et al. 2020). In addition, theory and computation were combined in our study of the Minkowski functionals (Boelens and Tchelepi 2021a). For a 3D porous medium the Minkowski functionals are related to the pore volume, surface area, integral mean curvature, and the Euler characteristic (i.e., connectivity) (Boelens and Tchelepi 2021b). For thermodynamical properties derived from a free energy, the Minkowski functionals are used to provide a complete description of the geometrical parameter space of a system. Both classical density functional theory and molecular dynamics simulations showed that these functionals are useful to describe accurately capillary condensation under tight confinement in porous media (Simeski et al. 2021). This opens new opportunities to better understand the effect of topology on sorption phenomena and to upscale molecular scale simulations to the experimental scale.

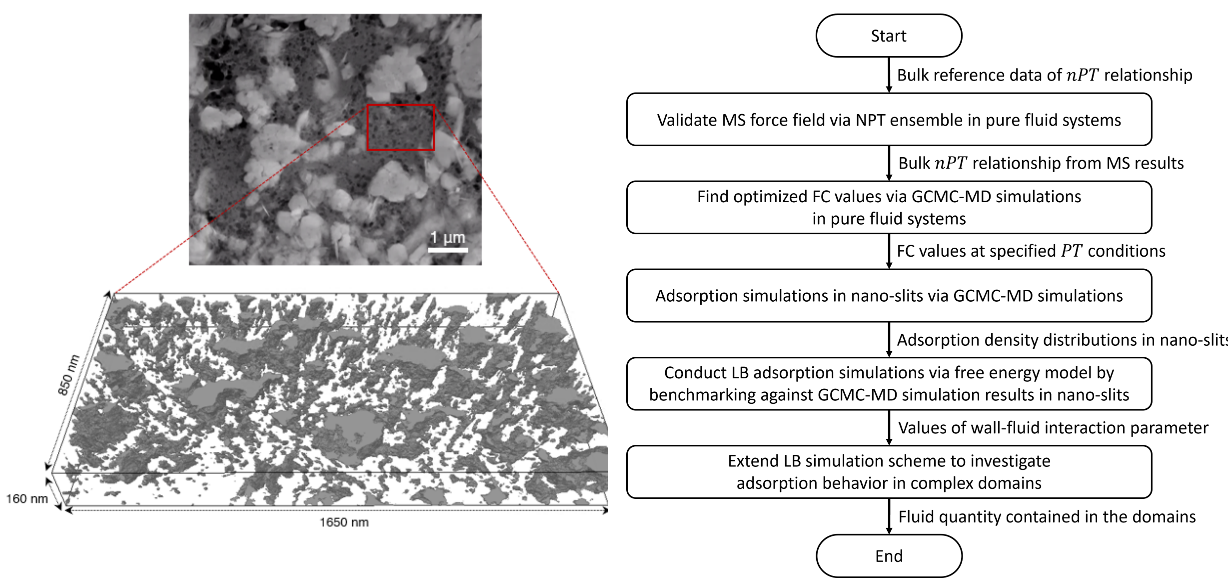


Fig. 8. Illustration of scale-translation framework (Liu et al. 2024): (a) Pore network of shale sample obtained via STEM (scanning transmission electron microscope) computed tomography and (b) flow chart of framework where MS is molecular simulation, GCMC is grand canonical Monte Carlo, MD is molecular dynamics, LB is lattice Boltzmann. The framework is capable of simulating transport on STEM images.

6. Other Impacts

Other notable accomplishments of CMC-UF include (i) extensive training opportunities for students in the geosciences and (ii) the collection, curation, and publication of unique image datasets as detailed in the Products section. CMC-UF had a nonscientific goal to create a highly trained, diverse, and empowered scientific workforce whose members possess depth in multiple areas sufficient to collaborate across geoscience and engineering science fields. Our collaborators include graduate students, postdoctoral scholars, and research staff. The table below summarizes the number of trainees supported throughout the lifetime of CMC-UF and gives some details on the succeeding professional positions that they filled.

Table 1. Summary of trainees.

	No. of Alumni	Notable next positions
Graduate students	42	Faculty: T.S. Alshafloot Postdoc: J. Sun, B. Medina Rodriguez (subsequently faculty), Y. Wang (subsequently faculty) US Gov't Lab: K. Guan, K. Rehmeier (nee Covington) Employment in Industry: Y. Aitosaffah, Y. Elkady, A. Singh, F. Guo, J. McKinzie, M.P. Murugesu Progressed into PhD: J. Bracci, R. T. Garza, Y. Perez-Claro, M. Sodwatana
Postdoctoral scholars	10	Faculty: B. Ling, C. Zahasky, H. Khan, B. Medina Rodriguez Postdoc: A. Kamali Asl, T.Kurotori
Technical staff	9	Faculty: Y. Mehmani
Undergraduate researchers	3	

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