GT MAP: the first workshop on Material

Tentative Schedule

Aug 17 (Wednesday)	Aug 18 (Thursday)	Aug 19 (Friday)
9:30 **Lowengrub (UCI)**	9:30 **Wang (MSE)**	9:30 **Erturk (ME)**
10:20 *coffee break*	10:20 *coffee break*	10:00 **Chow (CSE)**
10:40 **Suryanarayana (CE)**	10:40 **Goldbart (Physics)**	10:30 *coffee break*
11:10 **Kalidindi (ME)**	11:10 **Garmestani (MSE)**	11:00 **Fedele (CE)**
11:40 **Peng (EAS)**	11:40 **Ayazi (ECE)**	11:30 **Bracco (EAS)**
12:10 *lunch (on your own)*	12:10 *lunch (on your own)*	12:00 *lunch (on your own)*
1:30 **Lowengrub (UCI)**	1:30 **Wang (MSE)**	1:30 **Paaby (Biology)**
2:20 *coffee break*	2:20 *coffee break*	2:00 **Nenes (EAS)**
2:40 **Yavari (CE)**	2:40 **Wilkinson (Chem.)**	2:30 *end of the workshop*
3:10 **Kindermann (Phys.)**	3:10 **Ratcliff (Biology)**	
3:40 **Rimoli (AE)**	3:40 **Yunker (Physics)**	
4:10 **Cvitanovic (Phys.)**	4:10 **Kim (Physics)**	
Social Dinner 6:00	Informal discussion 4:45-5:15	

August 17, 2016 (Wednesday)

9:30 **John Lowengrub (UCI Math)**

Title: **Mathematical and Computational Modeling of Graphene Growth**

Part I. Single Layers (first talk 9:30AM)

Part II. Multilayers (second talk 1:30PM)

Abstract: The epitaxial growth of graphene on copper foils is a complex process, influenced by thermodynamic, kinetic, and growth parameters, often leading to diverse island shapes including dendrites, squares, stars, hexagons, butterflies, and lobes. We introduce phase-field models that provide a unified description of these diverse growth morphologies and compare the model results with experiments. We develop a minimal microkinetic model in order to relate the deposition rate with the partial pressures, to assess the importance of the different chemical species that might attach to the graphene edge. We also build a model for the kinetic coefficient, in this multiple species context. Our main assumption is that different species attach depending on the decoration of hydrogen on the interface, and hence their respective attachment- detachment coefficients should depend on this decoration. Our model explicitly accounts for the anisotropies in the energies of growing graphene edges, kinetics of attachment of carbon at the edges, and the crystallinity of the underlying copper substrate (through anisotropy in surface diffusion), and the complex island morphologies. We consider

both single and double layer islands. We show that anisotropic diffusion has a very important, counterintuitive role in the determination of the shape of islands, and we present a "phase diagram" of growth shapes as a function of growth rate for different copper facets. Our results are shown to be in excellent agreement with growth shapes observed for high symmetry facets such as (111) and (001) as well as for high-index surfaces such as (221) and (310).

10:40 **Phanish Suryanarayana (CE)**

Title: **Towards large and fast Density Functional Theory Calculations**

Abstract: Electronic structure calculations based on Density Functional Theory (DFT) have been remarkably successful in describing material properties and behavior. However, the large computational cost associated with these simulations has severely restricted the size of systems that can be routinely studied. In this talk, previous and current efforts of the speaker to develop efficient real-space formulations and parallel implementations for DFT will be discussed. These include linear scaling methods applicable to both insulating and metallic systems.

11:10 **Surya Kalidindi (ME)** and David Brough

Title: **Practical multiscale approaches for heterogeneous material systems using Materials Knowledge System**

Abstract: In recent years, our research group has formulated a new framework called Materials Knowledge Systems (MKS) for establishing highly accurate reduced-order models for bi-directional (i.e., homogenization and localization) exchange of salient information in hierarchical materials systems. These computationally efficient linkages are designed to capture accurately the microscale spatial distribution of a response field (e.g., strain field), of interest in the representative volume element (RVE) of a heterogeneous material, when subjected to an imposed macroscale change in the environment (e.g., loading condition, a temperature gradient). The viability and computational advantages of the MKS approach will be discussed and demonstrated with suitable case studies. The current challenges and opportunities in this research will also be discussed in detail.

11:40 **Zhigang Peng (EAS)**

Title: **Mining Seismic Wavefield**
Microseismic Detection and Future Development

Abstract: Recent advancemethese differences and show that in certain limits this theory permits an exact, analytic solution of the spectrum of twisted graphene bilayers. nts in seismic instrumentations around the world provide an unprecedented opportunity to unravel detailed structures of the Earths interior and decipher earthquake processes. While many earthquakes are routinely identified by analysts in seismic network centers, a significant fraction of them are still missing, especially during intensive earthquake swarms or major earthquakes sequences. These missing events could be detected by semi-automatic waveform matching method, which uses seismic data of existing events as templates to scan through continuous data for new events with high similarities. Here I report our groups recent efforts on systematic detections of missing microseismic events with this technique. These include forechocks/aftershocks of major earthquakes around the world, deep tectonic tremor along major plate boundary faults, and intermediate to deep focus earthquakes. These newly detected events help us to better understand the physical mechanisms of earthquake interactions from nearby to long-range distances, as well as deep geodynamic processes associated with plate tectonics. Finally, I describe future development in seismic instrumentation and computation, and potential challenges/opportunities within the field of seismology.

1:30 **John Lowengrub (UCI Math)**

Listed above.

2:40 **Arash Yavari (CE)**

Title: **Non-Riemannian Geometries and the Mechanics of Distributed Defects in Nonlinear Solids**

Abstract: In this seminar we present a geometric framework in which the residual stress field of nonlinear solids with distributed defects can be analytically calculated. As examples, we consider solids with distributed line and point defects. We first show that the nonlinear mechanics of solids with distributed defects can be formulated as a nonlinear elasticity problem provided that the material manifold where the body is stress-free is chosen appropriately. We discuss the relevance of the Riemann-Cartan-Weyl manifolds to a geometric description of dislocations, disclinations, and point defects. Using the method of Cartan's moving frames, we present some exact solutions in the nonlinear mechanics of dislocations.

3:10 **Markus Kindermann (Phys.)**

Title: **Twisted honeycomb multi-layers spectrum, transport, and topology**

Abstract: Graphene, a two-dimensional allotrope of carbon, has drawn much attention since its first experimental isolation. Much of this fascination stems from its exotic low-energy dynamics that is governed by the massless Dirac equation. In this talk I discuss how this dynamics is modified in multilayers of graphene or other planar, honeycomb crystals with an interlayer twist.

I will first discuss an effective long-wavelength theory of such multilayers, which is valid at small twist angles between the layers. Implications of this theory will be presented. For example, the theory predicts a spectral gap of graphene on hexagonal Boron-Nitride substrates, another instance of a honeycomb multilayer.

Next I will discuss the physics of commensurately twisted graphene bilayers. It will be demonstrated that in the case of even sublattice symmetry such bilayers are crystalline topological insulators.

Building on the two first parts of the talk I will then show that a long-wavelength theory can be constructed also for multilayers with large, incommensurate twist angles, provided that the angle is close to a commensurate one. The resulting theory is surprisingly similar to the one valid at small twist angle, but with important differences. I will discuss these differences and show that in certain limits this theory permits an exact, analytic solution of the spectrum of twisted graphene bilayers.

3:40 **Julian Rimoli (AE)**

Title: **On the nonlinear behavior of tensegrity structures under impact**

Abstract: The term tensegrity, derived from tensional integrity, refers to a certain class of structural systems composed of rigid bars and strings. Through adequate prestressing of their string members, tensegrity structures generally become mechanically stable, meaning that their load-bearing capability remains intact even after undergoing severe deformation. In this work, we study aspects related to the impact tolerance of tensegrity-based structures, and the implications this could have in the design of meta-materials for energy absorption applications. Traditional approaches for modeling the behavior of tensegrity structures have their origin on form-finding applications or on models based on their quasi-static behavior. As such, they generally assume that: (i) bars are perfectly rigid, (ii) cables are linear elastic, and (iii) bars experience pure compression and strings pure tension. In addition, a common design constraint is to assume that the structure would fail whenever one of its bars reaches the corresponding Euler buckling load. In reality, these assumptions tend to break down under impact events. We developed a reduced-order model for tensegrity structures capable of capturing their buckling and post-buckling behavior, and show how, under dynamic events, buckling of individual members of a tensegrity structure does not necessarily imply structural failure. Our research suggests that efficient structural design of impact-tolerant structures and meta-materials could be achieved by exploiting rather than avoiding the buckling of its compression members.

4:10 **Predrag Cvitanovic (Physics)**

Title: **Turbulence: how fat is it?**

Abstract: PDEs (such as Navier-Stokes) are in principle infinite-dimensional dynamical systems. However, recent studies support conjecture that the turbulent solutions of spatially extended dissipative systems evolve within an 'inertial' manifold spanned by a finite number of 'entangled' modes, dynamically isolated from the residual set of isolated, transient degrees of freedom. We provide numerical evidence that this finite-dimensional manifold on which the long-time dynamics of a chaotic dissipative dynamical system lives can be constructed solely from the knowledge of a set of unstable periodic orbits. In particular, we determine the dimension of the inertial manifold for Kuramoto-Sivashinsky system, and find it to be equal to the ''physical dimension' computed previously via the hyperbolicity properties of covariant Lyapunov vectors.

with Xiong Ding, H. Chate, E. Siminos and K. A. Takeuchi, arXiv.org/abs/1604.01859.

August 18, 2016 (Thursday)

9:30 **Zhonglin Wang (MSE)**

Title: **Piezotronics and Piezo-phototronics**

Abstract: Piezoelectricity, a phenomenon known for centuries, is an effect that is about the production of electrical potential in a substance as the pressure on it changes. For wurtzite structures such as ZnO, GaN, InN and ZnS, due to the polarization of ions in a crystal that has non-central symmetry, a piezoelectric potential (piezopotential) is created in the crystal by applying a stress. The effect of piezopotential to the transport behavior of charge carriers is significant due to their multiple functionalities of piezoelectricity, semiconductor and photon excitation. By utilizing the advantages offered by these properties, a few new fields have been created. Electronics fabricated by using inner-crystal piezopotential as a gate voltage to tune/control the charge transport behavior is named piezotronics, with applications in strain/force/pressure triggered/controlled electronic devices, sensors and logic units. This effect was also extended to 2D materials such as MoS2. Piezo-phototronic effect is a result of three-way coupling among piezoelectricity, photonic excitation and semiconductor transport, which allows tuning and controlling of electro-optical processes by strain induced piezopotential. The objective of this talk is to introduce the fundamentals of piezotronics and piezo-phototronics and to give an updated progress about their applications in energy science (LED, solar) and sensors (photon detector and human-CMOS interfacing).

[1] W.Z. Wu, X.N. Wen, Z.L. Wang Pixel-addressable matrix of vertical-nanowire piezotronic transistors for active/adaptive tactile imaging, Science, 340 (2013) 952-957.

[2] C.F. Pan, L. Dong, G. Zhu, S. Niu, R.M. Yu, Q. Yang, Y. Liu, Z.L. Wang* Micrometer-resolution electroluminescence parallel-imaging of pressure distribution using piezoelectric nanowire-LED array, Nature Photonics, 7 (2013) 752-758.

[3] Z.L. Wang Piezopotential Gated Nanowire Devices: Piezotronics and Piezo-phototronics, Nano Today, 5 (2010) 540-552.

[4] Q. Yang, W.H. Wang, S. Xu and Z.L. Wang* Enhancing light emission of ZnO microwire-based diodes by piezo-phototronic effect, Nano Letters, 11 (2011) 40124017.

[5] W.Z. Wu, L. Wang, Y.L. Li, F. Zhang, L. Lin, S. Niu, D. Chenet, X. Zhang, Y. Hao, T.F. Heinz, J. Hone, and Z.L. Wang Piezoelectricity of single-atomic-layer MoS2 for energy conversion and piezotronics", Nature, 514 (2014) 470-474.

10:40 **Paul Goldbart (Physics)**

Title: **Berry's transitionless quantum driving: Extensions and applications**

Abstract: Time-dependent quantum systems, if prepared in some instantaneous eigenstate of the system's time-dependent Hamiltonian, typically exhibit nonadiabaticity.

Said equivalently, they develop quantum amplitudes to be found in orthogonal instantaneous eigenstates. When the time dependence is slow, these amplitudes are small, as one can see explicitly, e.g., in the context Landau-Majorana-Zener model. Berry (2009) has shown how to construct a corrective Hamiltonian that suppresses quantum transitions out of instantaneous eigenstates, regardless of the pace of the time-dependence possessed by the original Hamiltonian: this is transitionless quantum driving. We discuss the extension of the concept of transitionless quantum driving to systems that possess exact degeneracies amongst their instantaneous energy eigenvalues and, as a result, exhibit the Wilczek-Zee (1984) nonabelian extension of Berry's connection (1984). We also discuss some of applications of transitionless quantum driving that should be realizable, experimentally. This talk is based on work done with Rafael Hipolito.

F. Wilczek and A. Zee (1984) Appearance of gauge structure in simple dynamical systems, Physical Review Letters 52, 2111-2114.

M. V. Berry (2009) Transitionless quantum driving, Journal of Physics A: Mathematical and Theoretical 42, 365303 [9 pages].

M. V. Berry (1984) Quantal phase factors accompanying adiabatic changes, Proceedings of the Royal Society of London Series A 392, 45-57.

11:10 **Garmestani (MSE)**

Title: **Inverse Materials Design and Homogenization using Green's Functions**

Abstract: The field of materials and microstructure design has progressed significantly in the past two decades. Materials and processing design methodologies effectively utilize the incomplete materials knowledgebase to link final product properties to initial microstructure using Greens function solution and correlation functions. Methodologies that can make the Inverse Materials Design a reality requires novel mathematical and computational frameworks and methodologies in addition to experimentally based knowledge creation to integrate computational-prediction and experimental-validation approaches. This talk will present current advances in multiscale computational materials frameworks based on Microstructure Sensitive Design and statistical homogenization techniques based on Greens function approaches. Microstructure representation and digitization using spectral techniques are at the heart of such methodologies. Application of the present methodologies in thermo-mechanical processing of advanced magnesium alloys, the effect of machining in Al and Titanium alloys and processing of textured silicon solar cells and solid Oxide Fuel Cells are discussed with respect to inverse methodologies.

11:40 **Farrokh Ayazi (ECE)**

TBA

1:30 **Zhonglin Wang (MSE)**

Title: **Triboelectric nanogenerator for self-powered systems and large-scale blue energy**

Abstract: Triboelectrification is an effect that is known to each and every one probably ever since the ancient Greek time, but it is usually taken as a negative effect and is avoided in many technologies. We have recently invented a triboelectric nanogenerator (TENG) that is used to convert mechanical energy into electricity by a conjunction of triboelectrification and electrostatic induction. As for this power generation unit, in the inner circuit, a potential is created by the triboelectric effect due to the charge transfer between two thin organic/inorganic films that exhibit opposite tribo-polarity; in the outer circuit, electrons are driven to flow between two electrodes attached on the back sides of the films in order to balance the potential. Ever since the first report of the TENG in January 2012, the output power density of TENG has been improved for five orders of magnitude within 12 months. The area power density reaches 500 W/m2, volume density reaches 490 kW/m3, and a conversion efficiency of 50% has been demonstrated. The TENG can be applied to harvest all kind mechanical energy that is available but wasted in our daily life, such as human motion, walking, vibration, mechanical triggering, rotating tire, wind, flowing water and more. Alternatively, TENG can also be used as a self-powered sensor for actively detecting the static and dynamic processes arising from mechanical agitation using the voltage and current output signals of the TENG, respectively, with potential applications for touch pad and smart skin technologies. The TENG is possible not only for self-powered portable electronics, but also as a new energy technology with a potential of contributing to the world energy in the near future.

[1] Z.L. Wang Triboelectric Nanogenerators as New Energy Technology for Self-Powered Systems and as Active Mechanical and Chemical Sensors, ACS Nano 7 (2013) 9533-9557.

[2] G. Zhu, J. Chen, T. Zhang, Q. Jing, Z. L. Wang* Radial-arrayed rotary electrification for high-performance triboelectric generator, Nature Communication, 5 (2014) 3456.

[3] Zhong Lin Wang,* Jun Chen, Long Lin Progress in triboelectric nanogenertors as new energy technology and self-powered sensors (invited review), Energy and Environmental Sci, 8 (2015) 2250-2282.

2:40 **Angus Wilkinson (Chemistry)**

Title: **Negative Thermal Expansion and Other Anomalous Properties in Metal Fluorides with Structures Related to that of ReO3**

Abstract: Materials with a cubic-ReO3 structure have long been suggested as good candidates for negative thermal expansion (NTE). Additionally, the simplicity of the cubic-ReO3 structure is appealing for studies focused on understanding the factors governing a materials properties. In 2010, the first ReO3-type material to display strong

NTE over a broad temperature range, ScF_3, was reported. Subsequently, we have prepared and examined by variable temperature and pressure diffraction experiments the effects of solid solution formation in Sc1-xMxF3 (M trivalent cation), and the properties of the cation ordered ReO3-type ABF6 (A divalent ion, B tetravalent ion). This work revealed an array of unusual properties including very strong negative thermal expansion, pronounced elastic stiffening on heating, strong softening on compression and temperature dependent porosity.

3:10 **Will Ratcliff (Biology)**

Title: **Exploring the evolution of multicellularity through experimental evolution**

Abstract: The origin of multicellularity was one of the most significant innovations in the history of life. Our understanding of the evolutionary processes underlying this transition remains limited, however, mainly because extant multicellular lineages are ancient and most transitional forms have been lost to extinction. We bridge this knowledge gap by evolving novel multicellularity in vivo, using bakers yeast as as model system. In this talk I will cover recent work examining: 1) how cells evolve to form multicellular clusters, 2) how these clusters become Darwinian individuals capable of adaptation, 3) how multicellular life cycles that include single-celled genetic bottlenecks arise in evolution (and why this is important), and 4) how nascent multicellular entities evolve to be more complex. Our approach, which allows for the study of macroevolutionary processes over microevolutionary timescales, demonstrates that multicellularity is less evolutionarily constrained than previously thought.

3:40 **Peter Yunker (Physics)**

Title: **Phase separation (and cooperation) in biofilms via contact killing: active matter through life and death events**

Abstract: By nature of their dense growth and extracellular metabolism, microbes face persistent cooperative dilemmas. Genetic assortment is the only general solution stabilizing costly cooperation, but all known mechanisms structuring microbial populations depend on the availability of free space, an often unrealistic constraint. Here, we describe a novel class of self-organization that operates within densely-packed bacterial populations. Through mathematical modeling and experiments with Vibrio cholerae, we show how killing adjacent competitors via the Type VI Secretory System (T6SS) precipitates phase separation via the Model A universality class of order-disorder transition, producing a new form of active matter mediated by killing rather than constituent mobility. We mathematically demonstrate that T6SS-mediated killing should favor the evolution of public goods cooperation, and empirically verify this prediction using a phylogenetic comparative analysis. This work illustrates the twin role played by the T6SS, dealing death to local competitors while simultaneously favoring the evolution of cooperation with kin.

4:10 **Harold Kim (Physics)**

Title: **Forces in DNA loops**

Abstract: DNA forms loops inside the cell for genome organization and gene regulation. Since these DNA loops undergo thermal fluctuations, they inevitably exert fluctuating forces on neighboring molecules, which may play important structural and functional roles in biology. In statistical mechanics, these forces are usually treated as an emergent quantity known as the thermodynamic force. But I argue that the thermodynamic force is only an average of fluctuating forces that individually may not resemble their average at all. Here, I will present a classical mechanical framework that relates these forces to curvatures of a hyper-dimensional manifold in phase space. Using this framework, the entire distribution of microscopic forces acting in the DNA loop can be obtained. I will highlight some features of these forces that defy our macroscopic intuition and discuss experimental results that may reveal some of these findings.

August 19, 2016 (Friday)

9:30 **Alper Erturk (ME)**

Title: **Next-generation smart structures and electroelastodynamic problems**

Abstract: This talk will review our recent efforts on the electroelastodynamics of smart structures for various applications ranging from nonlinear energy harvesting and acoustic power transfer to elastic wave guiding and vibration attenuation via metamaterials. The main focus will be placed on energy harvesting (theory and experiments) for small electronic components using piezoelectric transduction. The field of energy harvesting offers the promise of enabling self-powered electronic components for numerous applications ranging from conventional systems employing wireless sensor networks to next-generation components of the Internet of Things which will connect each individual to tens or hundreds of wireless devices for which periodic replacement or charging of batteries will be either too costly or cumbersome. In the context of energy harvesting, we will discuss how to exploit nonlinear dynamic phenomena for frequency bandwidth enhancement as an alternative to narrowband linear-resonant devices. We will also cover inherent nonlinearities (ferroelastic nonlinearity and intrinsic/extrinsic nonlinear dissipation), and their interaction with intentionally designed nonlinearities, as well as electrical circuit nonlinearities. Our recent efforts on phononic crystal-enhanced elastic wave guiding and harvesting, low-frequency broadband vibration attenuation via locally resonant metamaterials, contactless acoustic power transfer, nonlinear vibration and bifurcation suppression using nonlinear circuits, and exploiting size effects via strain-gradient induced polarization (flexoelectricity) in centrosymmetric elastic dielectrics will also be summarized.

10:00 **Edmond Chow (CSE)**

Title: **Very Fine-grained Parallelization of Preconditioning Operations**

Abstract: Massive concurrency is required in scientific and engineering algorithms in order to run efficiently on future computer architectures. High-end compute nodes already have hundreds to thousands of accelerator cores and core counts are anticipated to further increase. In this talk, we describe some new approaches for preconditioning operations, particularly incomplete factorizations and sparse triangular solves, that have much more concurrency than existing approaches. The main idea is to transform a problem into one that can be solved iteratively. By using asynchronous iterative methods, the coupling that must exist between processing units is obeyed, but can have much lower overhead than in the synchronous case.

11:00 **Francesco Fedele (CE)**

Title: **Explaining rogue waves may be simple after all**

Abstract: Since the 1990s, the modulational instability has commonly been used to explain the occurrence of rogue waves that appear from nowhere in the open ocean. However, the importance of this instability in the context of ocean waves is not well established. This mechanism has been successfully studied in laboratory experiments and in mathematical studies, but there is no consensus on what actually takes place in the ocean. In this work, we question the oceanic relevance of this paradigm. In particular, we analyze several sets of field data in various European locations with various tools, and find that the main generation mechanism for rogue waves is the constructive interference of elementary waves enhanced by second-order bound nonlinearities and not the modulational instability. This implies that rogue waves are likely to be rare occurrences of weakly nonlinear random seas. (joint work with F. Dias, J. Dudley, J. Brennan and S. Ponce de Leon, http://www.nature.com/articles/srep27715)

11:30 **Annalisa Bracco (EAS)**

Title: **Transport and mixing in the Gulf of Mexico: turbulence, oil, coral larvae and evolution**

Abstract: A physical ocean model simulating the circulation of the northern Gulf of Mexico and resolving submesoscale (0.1-10km) turbulence is used to investigate the oil patterns observed in the aftermath of the 2010 Deepwater Horizon spill and the connectivity between colonies of Leiopathes glaberrima, a black coral foundation species of deep-sea benthic communities. Results have important implications not only for targeting observational campaigns, but also for oil spill remediation and restoration efforts.

1:30 **Annalise Paaby (Biology)**

Title: **Cryptic genetic variation and the evolution of complex trait**

Abstract: Conditionally functional mutations are an important class of natural genetic variation, yet little is known about their prevalence in natural populations or how they mediate adaptive trajectories. In this talk I describe a vast reserve of cryptic genetic variation, alleles that are normally silent but which affect phenotype when the function of other genes is perturbed, in the gene networks of C. elegans embryogenesis. I find evidence that cryptic-effect loci are ubiquitous and segregate at intermediate frequencies in the wild. The cryptic alleles demonstrate low developmental pleiotropy, in that specific, rather than general, perturbations are required to reveal them. My findings underscore the importance of genetic background in characterizing gene function and provide a model for the expression of conditionally functional effects that may be fundamental in mechanisms of trait evolution.

2:00 **Athanasios Nenes (EAS)**

Title: **Representing and understanding aerosol-cloud interactions in climate models**

Abstract: Cloud droplets form upon pre-existing particles in the atmosphere ("aerosols"), and their modulation from pollution has profound impacts on the hydrological cycle and climate. Despite their importance, aerosol impacts on clouds constitute one of the most uncertain components of anthropogenic climate change, largely owing to the complex and multi-scale nature of aerosol-cloud interactions. This uncertainty motivated the development of sophisticated process-level microphysical schemes to represent particle-cloud interactions in climate model frameworks. Our research has largely focused on the development of such schemes that combine model reduction and observational constraints. The increasing complexity however makes the interpretation of climate model difficult, cumbersome and computationally expensive. We will demonstrate new approaches, based on adjoint sensitivity analysis, to quantitatively understand sources of variability in model simulations, and the spatiotemporal sensitivity of cloud parameters & processes to aerosol. This leads to a unique and effective way of understanding what is driving variability (here in cloud properties) with a limited number of simulations.