Built on LDRD Laboratory Directed Research and Development

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LDRD PROJECT NUMBER: 193373
LDRD PROJECT TITLE: Dynamic Mode Decomposition (DMD) of Solids
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ABSTRACT: Dynamic mode decomposition (DMD) is a method that has gained notoriety in the field of turbulent fluid flows as a method for decomposing the flow field into modes that could be further deconstructed to understand their influence on the overall dynamics of the system. Forays into solids and non-linear systems were considered, but not applied. In this work, DMD was applied for the first time to the heat-diffusion and reactive heat diffusion equations on a random particle pack of uniform solid spheres. A verification of a linear heat-diffusion test problem was successful, showing equality between the normal modes and Koopman modes obtained from DMD. Further application to a non-linear reactive system revealed stability limits of the underlying modes which are dependent on microstructure and chemical kinetics. This work will enable the development of reactive material models based on further analysis using DMD to quantify the statistical dependencies of transient response on microstructural characteristics.

INTRODUCTION:

As mesoscale modeling grows in importance and fidelity, the need to transfer the richness of statistical data present in these simulations is gaining recognition. To date mesoscale simulations have mainly been used to investigate certain aspects of the hot spot formulation process, focusing on the relative importance of different forms of energy deposition. As simulation domains have gotten larger, and approached the scale of hot spot transition to steady detonation, a more complete picture of the process has emerged. Full 2D or 3D state fields are now accessible from the moment of impact (due to mechanical, optical, or thermal means), to the creation and growth of hot spots and ultimately detonation. The volume of data available is large considering that statistical relevance requires that multiple iterations of a single microstructure, and many different microstructures need to be analyzed in order to get a clear picture of the governing physics of the process.

While much effort in discovery has been expended in finding way to “bridge scales” from molecular dynamics or atomistic scales to the continuum, the same emphasis has not been placed on bridging the mesoscale to the continuum. A particular physical process of interest in this area is the continuum of energetic material ignition processes, where a stimulus leads to energy localization at the mesoscale (for energetic materials this is the scale of particles, particle interfaces, pores, etc.) which leads to local reactions, which in turn leads to coalescence of reaction sites and either a steady detonation, or when heat losses dominate, a quenched or failed ignition. An idea that has been put forward as part of this exploratory LDRD is to bridge those scales through comprehensive mesoscale simulations leading to models that can capture the detailed build up to detonation in a statistical sense. In order to do this, methods must be developed to that are capable of efficiently translating highly coupled and non-linear data into the microstructure to response relationships that are needed for scale bridging.

For this LDRD, a possible method was outlined in our proposal that involved verifying the feasibility of using dynamic mode decomposition in coupled mechanical/reactive simulations. Dynamic mode decomposition is a technique published in 2010 (Schmid 2010), that was originally applied in problems of fluid flow, specifically in cases where unsteady periodic structures were present. Although not considered initially, shock physics problems are candidates for this treatment since at high pressures these solids behave like fluids, however the complicated nature of coupled physics problems (e.g., impact and transition to detonation) are currently an active area of research. Another motivation for this particular method is that for linear systems such as simple mass spring dashpot dynamics, or the diffusion of heat through a continuum or system of particles. This allows for a one to one validation of the method on a simple system, to which more complicated physics can be added. This report will describe in detail the dynamic mode decomposition method, the linear example problem, the application of the method to the problem, and the results of addition of non-linear physics to the example problem.

DETAILED DESCRIPTION OF EXPERIMENT/METHOD: Dynamic mode decomposition is a theory recently developed as a novel way of studying the field of high Reynolds number (turbulent) fluid flow. Decomposition analysis of these systems is interested in understanding the structures that greatly affect the dynamics of the fluid flow. "Decomposition" in this sense refers to the fact that the goal is to obtain a set of functions or modes that when superposed give the full flow field. Where DMD differs from previous approaches is in the basis that the flow is projected onto. Other methods project onto a basis of interest, or an orthogonal basis, where DMD employs operator theory to project onto a basis made up of eigenfunctions of a the linear Koopman operator (or the composition operator). One benefit of this approach is that the Koopman modes obtained from DMD on linear systems are identical to the normal modes obtained through a classical linear analysis (Mezić 2013).

Although our ultimate goal is to understand the effects of microstructure on real systems, it is not clear at this point how the results from DMD on such a problem would be interpreted. Before tackling the much more complicated problem of high strain rate simulations on non-linear solids, the DMD algorithm needs to be verified on a problem for which classical solutions exist. The problem chosen was thermal diffusion through a random particle pack which was subjected to a step function in temperature at each particle. The particle pack of uniformly sized spheres was generated using grain scale LAMMPS, and consisted of a square domain of around 1000 particles with periodic boundary conditions. Analysis of this system is greatly simplified by employing a directed graph approach, where each particle is represented as a vertex, and any neighboring particles that are in contact with a specific particle are connected through edges. This allows the whole domain to be represented in matrix form, and the heat diffusion equation can be solved by defining the transition rate matrix for the system.

While verification of the linear system is a necessary first step, extension to non-linear systems is absolutely critical to the ultimate application to dynamics of real material systems. The approach chosen to introduce non-linear physics into this system was to add uniform single step chemistry to every particle in the domain. With normalized, temperature dependent Arrhenius kinetics in

place throughout the domain, the desired non-linearity was obtained, and could be seen through "thermal runaway" at each particle. The simple addition of chemistry to the problem not only results in an abstraction from the interpretation of the linear system, but also results in a bifurcation of the solution space. With chemistry, two types of solutions are now possible, 1: the stable or homogeneous temperature solution observable in late time and is similar to the linear late time solution, and 2) the unstable or runaway temperature solution. This unstable solution was the focus of the Semenov and Frank-Kamenetskii problems, where rates of heat generation and heat diffusion are studied in relation to reactive solids and material sensitivity.

RESULTS: We model thermal conduction and reaction in a particulate material as a discrete form of the Frank-Kamenetskii (reaction-diffusion type equation) equation. The specific equations we investigate can be written as

$$\frac{\partial T_i(t)}{\partial t} = \sum_{j \neq i} L_{ij} T_j(t) + \frac{Q c_0 k_0}{\rho c_v} \exp\left(-\frac{U}{R T_i}\right)$$

with periodic boundary conditions. Here, T_i is the temperature of the i^{th} vertex (particle) and L_{ij} is the conduction matrix which describes a reduced-order model of thermal conduction between vertices, the rest of the parameters are material properties (density, heat capacity, heat of reaction, activation energy, etc.) that describe the nature of the first-order chemical reaction modeled by the last term on the RHS. This approach allows us to capture the relevant qualitative physics while keeping the mathematics simple and clear enough for analysis. Thus, this approach gives a direct connection to the well understood linear case by ignoring the last term on the RHS and allows for systematic variation of the strength of the nonlinearity by varying the parameters used in the reaction term. The results exhibited in this section are for a single set of parameters entering the equation above. The particle microstructure is obtained via Discrete Element Simulation of monodisperse frictionless spheres. Roughly 1000 particles are isotropically compressed and allowed to relax to obtain a well-controlled amorphous or random structure. No particle yield or fracture occurs as the intra-particle stresses remain within the linear elastic regime. The particle contact network defines the graph, and the particle-particle contact areas define the weights on the graph edges used to form the conduction matrix in the discrete equations analyzed in this section.

For the linear case, i.e. without the reaction term in the above equation, we can simply use standard algorithms to find the eigenvalues and eigenvectors of the linear operator, Lij. Following standard practice (Rowley, Mezić et al. 2009), the Koopman modes can be obtained from the DMD algorithm. In the linear case, it is known that these are identical to the normal modes. We confirm this result for the current case of thermal conduction in particulate materials with random mesostructure. An example of the results for eigenvectors (Koopman modes) can be seen in Figure 1, while eigenvaules can be seen in Figure 3 (orange data).

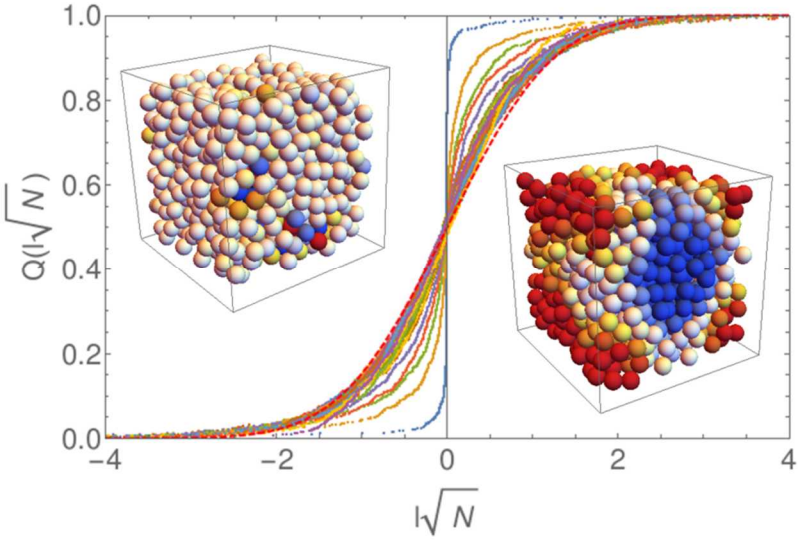

Figure 1: Eigenvector statistics (CDF of components in various eigenvectors) for linear conduction operator for reduced-order network model of conduction in random particle pack. Insets show particles color coded based on the magnitude of their contribution to eigenvectors associated with large eigenvalue (upper left) and small eigenvalue (lower right).

Addition of the first-order reaction term to the conduction model introduces nonlinearity into the equations. Depending on the value of the parameters one may find multiple solutions and instabilities as is often the case for systems of nonlinear equations. Here, depending on the values on the parameters and initial conditions, one finds, in addition to the isothermal solution from the linear case, an instability associated with thermal runaway type phenomena. While modeling the final temperature accurately is not expected, the time to runaway can be reasonably approximated. Figure 2 demonstrates the type of results obtainable. In the inset, the total temperature of a 978 particle system is plotted as a function of time for 978 different initial conditions (defined by giving a unit impulse separately to each particle in the system). As can be easily seen, the temperature of the system is stable for some time, which varies depending on which particle is chosen to receive the initial impulse, before it increases rapidly. If the "time-to-runaway" is defined, somewhat arbitrarily, as the time when the temperature surpasses twice the initial impulse, the statistical distribution of said quantity can be ascertained as displayed via the histogram in the main panel of Figure 2.

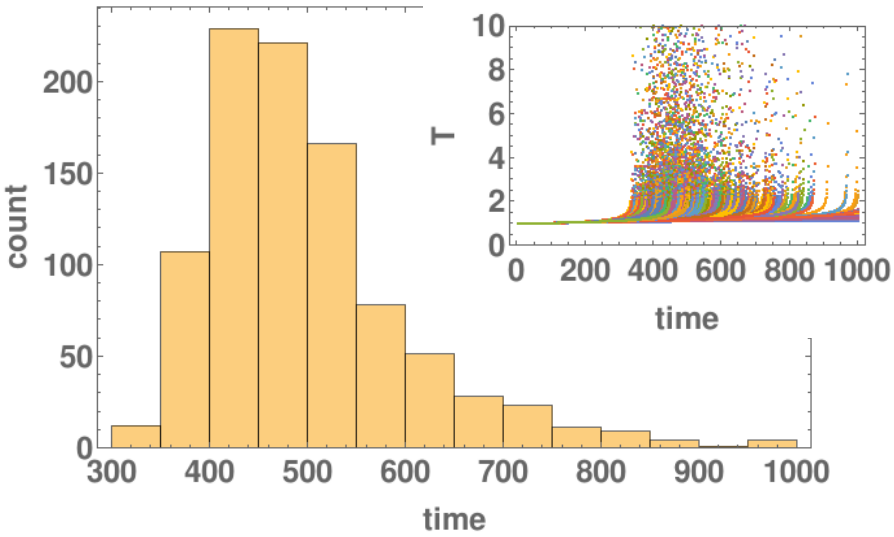

Figure 2: Histogram of time-to-runaway (see text) as a result of unit impulse given separately to each particle in the system (978 total). Inset: total system temperature versus time resulting from each unit impulse initial condition.

With the above nonlinearity in the system, the ability of the DMD approach to approximate the Koopman eigenvalues and modes can be tested, given that the Koopman operator is a linear operator even though the underlying dynamics are nonlinear. Figure 3 is the proof of concept for this approach in a solid material with reaction-diffusion type nonlinear dynamics. Here the eigenvalues, λ_i, for the conduction matrix are plotted from smallest to largest. In fact, λ_i-1 is plotted to illustrate contrast between the linear and non-linear systems. For the linear system the eigenvlaues of the evolution operator all fall in the stable (λ-1 $\leq$ 0) regime while the Koopman eigenvalues obtained from the standard DMD algorithm on the nonlinear problem show values above and below zero. The values less than zero can be associated with stable modes related to vectors corresponding to the Koopman eigenvalues.

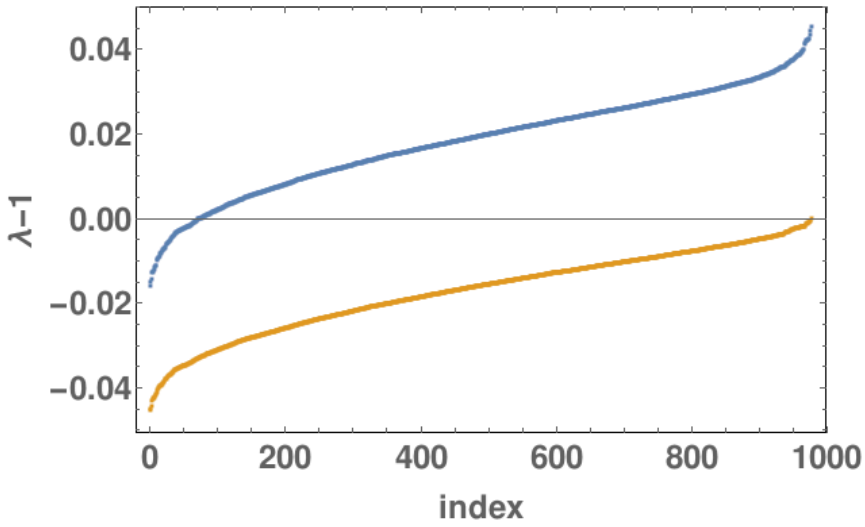

Figure 3: Koopman Eigenvalues obtained from standard DMD algorithm for the linear (orange) and nonlinear (blue) cases considered in this section (see text).

DISCUSSION: The approach taken here, for which this work serves as a proof of concept, has broad implications. Indeed, there have been recent attempts to formalize this kind of approach under the description of "Applied Koopmanism" (Budišić, Mohr et al. 2012). Hence, a number of applications may find useful concepts here. In particular, for the types of systems of closest relation to this work, it is expected that the span of the modes associated with the stable regime of Koopman eigenvalues defines the metastable basin of attraction for the isothermal solution to the equations, while the rest are associated with unstable, or run-away, ignition-type modes. It may be possible that these modes provide the access for characterization of microstructures and subsequent control and design of mesostructure-informed performance. Some hints of this possibility can be found by looking at the eigenvector contribution colored particle fields for stable and unstable solutions, where statistics can be obtained on contact networks near hot-spots. Additionally, this approach opens interesting avenues into powerful theoretical machinery in the area of nonlinear dynamical systems and non-equilibrium statistical mechanics. While it remains to be seen just how practical these concepts can be made for applications of interest, it is intriguing to recognize, for example, that the largest eigenvalue of the Perron-Frobenius operator (the adjoint of the Koopman operator) represents the so-called topological pressure. This may also be interpreted as a dynamical free energy in analogy to thermodynamics. It plays a key role as it is related by Legendre transform to the dynamical entropy, or large deviation function which describes the statistics of large deviations (deviations from standard Gaussian statistics), which are characteristic of heterogeneous materials. This may have profound implications for questions of uncertainty quantification and materials reliability.

However, there are a number of issues that remain open. The first is to complete the effort initiated here by performing a systematic study of the effects of nonlinearity due to the chemistry model employed. Of particular interest is to carry through the type of theoretical analysis described in the previous paragraph with a view to providing design guidance or uncertainty quantification. As a proof of concept, a single choice of chemistry mechanism, and a single parameterization of that chemistry sufficed to show the value of the analysis in relation to stable and unstable modes. However, for applications, a much more detailed and quantitative understanding of how sensitive the method is to changes in the parameterization is needed. Also, looking into the form of the chemistry model and just how well this particular model captures actual phenomena is to be determined. Another area that remains to be explored is the microstructure variability. Again, for proof of concept, a single microstructure is sufficient, but a hallmark of heterogeneous materials is not only their local variability, but their instance variability. To probe this, several different microstructures will need to be generated, and systematic analyses performed. These studies will at the least, provide a sense of the uncertainty in a plot of the eigenvalues, which when centered around the stable/unstable threshold (zero value in Figure 3), can yield information on necessary safety margins.

The previous discussion highlighted some necessary steps towards verifying this approach in the defined context of linear and non-linear reaction-diffusion on random particles packs. The aim is for this to be applied to mesoscale simulations of energetic materials. These represent complex multi-physics simulations involving high strain rate solid deformation shock physics with complex chemical reactions. Because of the extreme conditions that result in shock waves propagating in solids, the physics is often “hydrodynamic”, or fluid like, due to the decreased role of material strength in the dynamics. Because of this, there may be some similarities to turbulent fluid flows where DMD has found fruitful application. When shock waves approach a material heterogeneity such as a pore or particle inclusion, the disparate states of the shock wave in the material and at the interface between the material and the heterogeneity can create dynamic structures that resemble fluid vortices. A “jet” is often produced at the leading edge of pores that impacts the trailing edge of the pore, and the pore areas to either side of this jet are regions of high vorticity (see Figure 4). Despite these apparent similarities, much remains unclear as to how far the analogy will hold in addition to the aforementioned challenges of making the theoretical machinery applicable at a practical level.

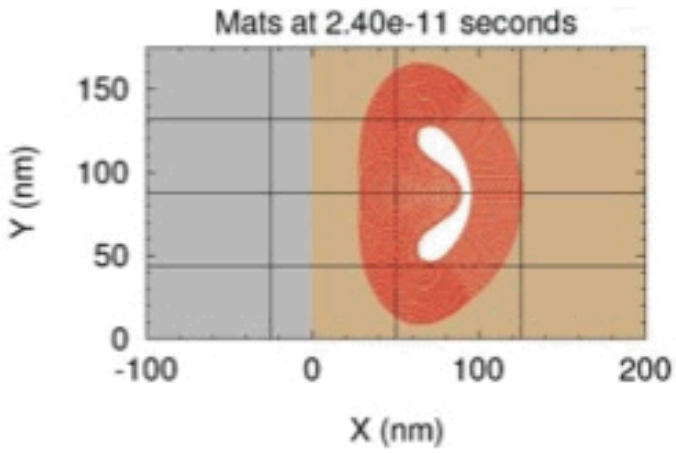

Figure 4: Representative simulation image of a collapsing pore due to shock passage. A jet has been formed and is approaching the trailing edge of the pore. The remaining pore regions to either side of the jet will develop significant vorticity.

ANTICIPATED IMPACT: The results of this project will provide immediate impact due to the fact that the verification of the methods to non-linear problems was an essential enabling step. The purpose of the project was to develop a toolset to numerically implement the dynamic mode decomposition theory, and furthermore to verify that the same toolset could be used in a non-linear problem. In the immediate term, the results obtained allow for a seamless continuation of the long term plan. Aspects of the long term plan that will begin immediately are 1) Performing due-diligence on the obtained results for both linear and non-linear systems by investigating the variability in the crossover between stable and unstable modes due to changes in either microstructure or chemistry, 2) preparation of a journal manuscript and submission to a high impact publication, and 3) application of the DMD toolset to other non-linear multiphysics problems such as the creation of hot spots in shock impacted material and subsequent heterogeneous chemistry.

Using the ongoing results obtained over the course of this project, an LDRD idea was created, and a subsequent proposal was written for review by the LDRD Engineering Sciences investment area team. The proposal “Pushing Continuum Reactive Capabilities through Novel Sub-Grid and Statistical Methods” was accepted in FY16 and is set to begin in FY17. This work was a critical step for the acceptance of this proposal, due to the central nature of the DMD method in the project plan. In this full LDRD proposal, DMD will be used on a varied set of microstructures that are representative of materials of interest to SNL. Through the application of DMD to these microstructures, the form of the dependence on microstructure will be determined, and this will ultimately allow for the predictive simulation of response from a priori knowledge of the microstructure. Across the labs, a push for a physics based ability to tackle the new problems in stockpile stewardship has been sought after. In particular, researchers and managers

at the explosive components facility (ECF) have led the push for a science based design and surveillance capability, where physics based models will play a central role. The results of this project, and the proposed LDRD are directly aimed at providing this capability for energetic materials.

There are many questions of both scientific and programmatic interest that this project will ultimately enable answering. The question that is the driver and archetypical problem for current efforts is that of explosive detonation threshold. In a threshold experiment, an explosive is first pressed to a specified density. The explosive pellets are then subjected to varying levels of shock pressure and duration. At a given value of one of the shock variables where detonation is known to develop, the failure threshold is determined by varying the other parameter until a successful detonation is not achieved. The question that current physics models cannot address currently is why the experimentally determined threshold curve changes with different microstructures at the same density. By building in the effects of microstructure from the start this question may finally be resolved.

Another question that arises is that of why aged materials behave differently in terms of their sensitivity to external stimuli. While modified chemistry is one obvious culprit for this phenomenon, changing microstructure over time is another. By enabling microstructure aware models, this project will directly impact the approach to analyzing this phenomenon.

While the impact to current and mid-term technology gaps has been the primary focus of this work, it is anticipated that this project has further reaching impact due to its general premise; where there exists a strong microstructure and response dependence, these effects must be treated properly in order for a predictive capability to succeed. There are many other areas where microstructure is known to be a dominating factor in observable behavior. Some of these areas are 1) Thermal runaway in slow cookoff environments, 2) propagation of deflagration waves in pyrotechnic materials, 3) the creation and propagation of cracks, 4) the “damage” introduced in state cyclical environments, and 5) the response of materials to extreme fluid or thermal environments.

Interest in these tools is anticipated to extend beyond the DOE and its applications. Anticipating this need, the team members have begun discussions on the best way to involve other partners within the DOE and DOD complex, and also in industry. The team anticipates that in FY20 appropriate collaborations will be in place to continue to further development of this work in the application space.

CONCLUSION: A dynamic mode decomposition toolset was implemented and applied to a thermally stimulated random particle pack for the first time. This work was motivated by a general need to quantify and understand how microstructure characteristics affect the dynamic behavior of materials. DMD was first applied to the linear case of thermal diffusion following local step impulses in temperature, and was subsequently applied to a non-linear case where temperature dependent chemistry resulted in thermal runaway conditions. Verification of the

linear case was accomplished by comparison to a classical analysis on the same data; this yielded identical results for Koopman and normal modes. The novel application of DMD to the non-linear solid problem followed, and was the first study of its kind. This study is without a classical analog, and so the interpretation of the results represented another first. It was found that the normalized Koopman values, which are analogous to eigenvalues in linear systems, represent the stability of the system. Unit Normalized Koopman values above zero represent unstable modes that will end in a runaway event where homogenous solutions are not possible, while values below zero represent stable, single temperature solutions.

Several potential applications were identified where these results may have impact and benefit researchers. The immediate application is in the area of energetic materials reactive burn modeling. Burn models that are microstructure aware are sought after because current methods are not able to accurately reproduce the observed threshold behavior of explosives. The methods being considered for this task depend on an intimate understanding of how microstructural details affect the local state of materials undergoing a dynamic event. This work will enable the acquisition of that understanding in a quantitative sense, which will enable the formulation of microstructure aware reactive burn models. Several other areas of application were enumerated, and these are generally described as any phenomena where the microstructure/response relationship is known to exist and can be quantified through detailed simulations or measurements. Funding is currently being sought through LDRD, DOD, and industry sources.

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