PRISM
NNSA CENTER FOR PREDICTION OF RELIABILITY, INTEGRITY AND SURVIVABILITY OF MICROSYS TEMS

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By
Purdue University
in collaboration with
University of Illinois, Urbana-Champaign,
University of New Mexico,
and
Vanderbilt University
July 2011
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EXECUTIVE SUMMARY

During the last few years, there has been a great deal of investment in the development of micro-electro-mechanical systems (MEMS) for civilian and defense applications. However, in order for MEMS to be included in weapons applications, they must satisfy stringent performance and reliability requirements. Despite significant effort, MEMS have not thus far been able to meet these criteria and experience unexpected failures, the reasons for which are poorly understood. If these problems could be solved, MEMS would find widespread deployment.

Purdue University, in collaboration with the University of Illinois, Urbana-Champaign, the University of New Mexico and Vanderbilt University, has established a center, PRISM: NNDA Center for Prediction of Reliability, Integrity and Survivability of Microsystems, to significantly accelerate the development of MEMS technologies through the use of predictive, validated science and petascale computing. The Center seeks to understand, control, and improve the long-term reliability and survivability of capacitive contacting RF MEMS by using multiscale multiphysics simulation, from atoms to micro-devices, to address fundamental failure mechanisms. Uncertainty quantification forms a central unifying theme of the center.

PRISM research is conducted under three Center thrusts, Contact Physics, Multiscale Modeling of Membrane Response, and Multiscale Modeling of Aerodynamic Damping. Two cross-cutting technology thrusts also support PRISM research, including Computational Science and Engineering (CSE), and Uncertainty Quantification Science. A substantial Center effort addresses verification, validation and uncertainty quantification issues specific to multiscale multiphysics simulations in microsystems. A strongly-leveraged experimental program is being conducted at Purdue’s state-of-the-art Birck Nanotechnology Center to augment published data with validation-quality measurements and to develop a first-of-its-kind validation database for uncertainty quantification in microsystems. A 5-year simulation program is underway, starting with system simulations based on continuum physics, adding complexity yearly, and culminating in petascale simulations of RF MEMS lifetime under both normal and accelerated testing conditions.

During Year 3, four important milestones were met. First, structural response simulations under the action of fluid damping and electrostatic actuation with and without contact were conducted to compute static and dynamic pull-in as well as multi-cycle contact. Good agreement with measured PRISM Generation 2 pull-in voltage as well as with measured deformation-versus-voltage curves was obtained, and with quantified uncertainty. The second milestone was the simulation of dielectric charging under sustained contact. A new multi-trap depth dielectric charging model was developed and was calibrated to charging data on a metal-insulator-metal (MIM) capacitor. Simulations of charging in the MIM capacitor were performed, and they identify the trap depth and barrier height as the primary determinants of prediction uncertainty. The third milestone for Year 3 was the prediction of long-term creep with quantified uncertainty. A Coble creep model for second-stage creep in the nickel membrane was developed. It was used in MEMOSA to predict the evolution of gap versus time for a frogleg varactor for which long-term creep data have been measured at Purdue. A Bayesian network approach was adopted, and Bayesian calibration of creep constants and subsequent analysis indicate that model-form error, possibly resulting from the neglect of residual stress, is significant. Under the fourth milestone, we developed a coarse-grained solver for system simulation based on the work performed in Year 2. Lifetime predictions using the model were performed, coupling elastic membrane response, electrostatics, fluid damping and dielectric charging, and the major sensitivities of the time-to-failure to system inputs were identified. Furthermore, the coarse-grained model was used to develop and evaluate multi-scale coupling
and uncertainty propagation during a single-event contact simulation of dynamic pull-in and pull-out and for long-term creep prediction.

A critical advance in Year 3 has been the development of a Bayesian network approach to system-level uncertainty quantification. Uncertainty quantification in PRISM switch simulations must account for multiple length and time scales, and involves a variety of physics, as well as simulations and experiments of varying levels of fidelity. The methodology integrates the contributions of input variabilities, data uncertainty (experimental and other sources) and model uncertainty and error at multiple levels of the system hierarchy. The components of this effort include model calibration, model validation, error and uncertainty quantification, confidence assessment in system-level prediction, and sensitivity analysis. We have demonstrated the use of Bayes networks in developing a calibrated creep model in MEMOSA-FVM for frogleg MEMS devices and for calibrating residual stresses in PRISM Generation 5 devices using experimentally-measured pull-in data.

A large number of improvements to the physical models in MEMOSA were made during Year 3. A central advance was the development of a mesoscale contact model incorporating atomistic inputs for surface roughness and elastic constants, and which admits an elasto-plastic response. The contact model was implemented in MEMOSA-FVM and in our coarse-grained solver, and milestone simulations using it were performed. Another important contribution was the development of a multiscale dielectric charging model for amorphous silicon nitride incorporating multiple trap depths, and informed by molecular dynamics and density function theory computations of defect levels and their distributions. A new methodology was developed for extracting model constants from metal-insulator-metal (MIM) charging experiments. Research on the inclusion of grain size and orientation in creep modeling continues. Refinement of our near-contact fluid damping model was conducted and points to the inadequacy of small-amplitude damping models in the literature for capturing the fluid damping behavior close to impact.

Enhancements to the numerical algorithms underlying MEMOSA were also made in Year 3. These include the development of a plate element model in MEMOSA-FVM to facilitate the efficient and accurate structural analysis of extremely high aspect ratio membranes. The plate element model supports geometrically complex thin structures, and has been integrated with our immersed boundary method to facilitate the simulation of fluid-structure-electrostatics problems. Furthermore, a creep model was developed in MEMOSA-FVM and may be used either in conjunction with a complete structural solution or with the plate element model. A residual stress model was also incorporated in MEMOSA-FVM. In addition, the ES-BGK implementation in MEMOSA-FVM was completed, and extensive verification of all new models, numerics and software has been conducted. In Year 3, improvements to the parallel scaling of MEMOSA-FVM were made, including the completion of the SPIKE algorithm implementation. MEMOSA-MPM was enhanced through the inclusion of a J2 plasticity model, and significant scaling improvements were made which allow the solver to scale efficiently to 1024 cores and more. PuReMD, our reactive molecular dynamics solver, was enhanced to support force field optimization. Furthermore, improvements to the charge equilibration algorithm in PuReMD continue to be made, including the development of a SPIKE based pre-conditioner. The MEMOSA-UQ environment was enhanced to include adaptive collocation, and work on the development of a compact model database, an essential ingredient of Bayesian network analysis, was initiated.

During Year 3, extensive experimental work was conducted to support validation efforts. Damping measurements across a range of pressures were completed for the PRISM device. Long-term creep measurements of frog-leg devices were conducted to support calibration of the creep model in MEMOSA-FVM. Generation 5 PRISM devices were fabricated, and geometric measurements of the device were made to support the development of input probability distributions of geometric parameters for our modeling efforts. Furthermore, measurements of the elastic modulus of the PRISM membrane as
well as the first experiments on contact and bounce were initiated. Microstructural characterization of the membrane structure was conducted to inform the atomistic and mesoscale material modeling effort.

A comprehensive educational program was conducted in Year 3, including workshops, a lively seminar series, additions to the Computational Science and Engineering program, and a student internship program at the national laboratories. A 1-credit seminar class entitled “Introduction to Uncertainty Quantification” was taught by PRISM researchers during Fall 2010. The MEMShub web portal was enhanced to disseminate research, software, experimental data and pedagogical materials to the MEMS community, and continues to be populated with content. The most recent additions to MEMShub include an improved coarse-grained solver for MEMS design and simulation, and the recorded video lectures from our uncertainty quantification seminar course.
List of Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>AFM</td>
<td>Atomic Force Microscopy</td>
</tr>
<tr>
<td>BTE</td>
<td>Boltzmann Transport Equation</td>
</tr>
<tr>
<td>BGK</td>
<td>Bhatnagar-Gross-Krook</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CSE</td>
<td>Computational Science and Engineering</td>
</tr>
<tr>
<td>DOE</td>
<td>Department of Energy</td>
</tr>
<tr>
<td>ES-BGK</td>
<td>Ellipsoidal-Statistical Bhatnagar-Gross-Krook</td>
</tr>
<tr>
<td>FVM</td>
<td>Finite Volume Method</td>
</tr>
<tr>
<td>gPC</td>
<td>Generalized Polynomial Chaos</td>
</tr>
<tr>
<td>IBM</td>
<td>Immersed Boundary Method</td>
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<tr>
<td>MD</td>
<td>Molecular Dynamics</td>
</tr>
<tr>
<td>MEMOSA</td>
<td>MEMS Overall Simulation Administrator</td>
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<tr>
<td>MEMS</td>
<td>Micro-Electro-Mechanical Systems</td>
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<tr>
<td>MIM</td>
<td>Metal-Insulator-Metal</td>
</tr>
<tr>
<td>MPM</td>
<td>Material Point Method</td>
</tr>
<tr>
<td>MPI</td>
<td>Message Passing Interface</td>
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<tr>
<td>NNSA</td>
<td>National Nuclear Security Administration</td>
</tr>
<tr>
<td>NSSJ</td>
<td>Navier-Stokes Slip Jump</td>
</tr>
<tr>
<td>PIRT</td>
<td>Phenomena Identification and Ranking Table</td>
</tr>
<tr>
<td>PFMM</td>
<td>Phase Field Micromechanics</td>
</tr>
<tr>
<td>PRISM</td>
<td>Prediction of Reliability, Integrity and Survivability of Microsystems</td>
</tr>
<tr>
<td>RF</td>
<td>Radio Frequency</td>
</tr>
<tr>
<td>SEM</td>
<td>Scanning Electron Microscopy</td>
</tr>
<tr>
<td>SII</td>
<td>Secondary Ion Image</td>
</tr>
<tr>
<td>TEM</td>
<td>Transmission Electron Microscopy</td>
</tr>
<tr>
<td>UQ</td>
<td>Uncertainty Quantification</td>
</tr>
<tr>
<td>VALTS</td>
<td>Validation Testing Suite</td>
</tr>
<tr>
<td>VERTS</td>
<td>Verification Testing Suite</td>
</tr>
<tr>
<td>V&amp;V</td>
<td>Verification and Validation</td>
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</table>
1. INTRODUCTION
Over the last two decades, micro-electro-mechanical systems (MEMS) have demonstrated the potential to revolutionize the landscape of civilian and military communications, signal processing, and sensing. Integrated microsystems for monitoring and control of National Nuclear Security Administration (NNSA) stockpiles and new weapons systems are of critical national interest because they offer significant cost reduction and performance enhancement. Despite the increasingly widespread deployment of resonators, gyroscopes and digital light processing technologies in the commercial arena, the deployment of MEMS in military applications has been hindered by the lack of reliability, particularly for complex moving and contacting MEMS designs. In order for MEMS to be included in NNSA stockpiles, they must satisfy stringent performance and reliability requirements. MEMS must survive billions of cycles of operation, and must operate properly under dynamic impact conditions with acceleration/deceleration levels of up to 30,000g lasting milliseconds. Operating temperatures may vary from -50 to 80°C. Furthermore MEMS must function reliably even after they have been stored for long periods. Despite significant efforts in both the civilian and defense sectors, MEMS have not thus far been able to meet these criteria, and experience unexpected failures, the reasons for which are poorly understood. Consequently, there is little guidance to address these failures, and no obvious path to improvement. If MEMS could be made to function reliably long-term in adverse environments, they would find widespread use in NNSA weapons systems.

Purdue University, with its partners at the University of Illinois Urbana-Champaign (UIUC), the University of New Mexico (UNM), and Vanderbilt University, has created a Center for Prediction of Reliability, Integrity and Survivability of Microsystems (PRISM) to accelerate substantially the development of MEMS technologies for civilian and military applications. PRISM aims to significantly improve our understanding of the long-term reliability of MEMS and their survivability in harsh environments by simulating rigorously, and at multiple scales, the physics of failure, accounting for the coupled electrical, mechanical, thermal and materials behavior of MEMS, from atoms to devices. Advanced simulation software, encapsulated in an integrated simulation system, MEMOSA (MEMS Overall Simulation Administrator), is being developed by leveraging existing DOE codes and our own research codes, and developing new methodologies and software as necessary. Uncertainty quantification (UQ) is a critical component of PRISM research; UQ methodologies are being woven into the very fabric of our software so that our integrated software suite can quantify the cumulative uncertainty of all the constituent multiscale multiphysics components. An extensive program for verification and validation is underway which systematically addresses the multiscale multiphysics nature of the problem, and which is supported by a significantly-leveraged experimental effort being undertaken at Purdue’s state-of-the-art Birck Nanotechnology Center in collaboration with Sandia National Laboratories. At completion, PRISM will allow NNSA researchers to predict, understand, and alleviate MEMS failure mechanisms, and thus to improve their reliability and survivability.

This document is structured in the following way. Section 2 gives an overview of PRISM goals, its main technical thrusts, and the Center management structure. Section 3 lays out specific prediction goals and PRISM’s 5-year simulation milestones. Sections 4-9 summarize research accomplishments for the period April 2010-April 2011. Section 10 gives an overview of educational and outreach achievements. The remaining sections provide schedule and personnel information, and a list of Center publications.
2. CENTER OVERVIEW
2.1 Overarching Application

The focus of PRISM is on a single contacting radio frequency (RF) capacitive MEMS switch. The target system and its most important material and geometrical properties are shown in Fig. 2.1. This type of device is widely used for contact actuators and capacitive switches, and involves metal-dielectric contact. A fixed-fixed nickel membrane makes repeated contact with a dielectric contact pad. In the up state the switch presents a very small capacitance (0.03–0.1 pF) which allows the signal to travel through the transmission line (blue) with very low loss (<0.1dB up to 40GHz). On the other hand, in the down state, the suspended bridge contacts the dielectric layer forming a large capacitance (1–3 pF), which is an effective short circuit at high frequencies (>5–10 GHz). Consequently, the incident signal is reflected and the switch presents a high isolation (>15–30 dB).

During the last decade, significant work has been performed in improving switch reliability, and recent designs have begun to exhibit lifetimes of nearly a trillion cycles\textsuperscript{3,4} (i.e., a few months) in a laboratory environment and for low power levels (<100 mW). The primary failure mechanisms exhibited by this type of RF

![Figure 2.1: Target RF MEMS device. Applied bias causes the metallic membrane (gold) to close gap and make contact with the dielectric (brown) over a time scale of microseconds. The device is enclosed in a sealed enclosure containing nitrogen or air.](image)

<table>
<thead>
<tr>
<th>Problem</th>
<th>Description</th>
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<tbody>
<tr>
<td>Dielectric Charging</td>
<td>Caused by trapped charges in thin dielectric layers; causes uncontrollable changes of actuation voltage with time</td>
</tr>
<tr>
<td>Contact Area Damage and Current Channeling</td>
<td>Contact resistance increases with time even at low power probably due to strain hardening and change of chemistry. Surface roughness evolution due to contact and non-uniform distribution of traps causes preferred current paths to form, increasing surface damage.</td>
</tr>
<tr>
<td>Environmental Factors</td>
<td>High humidity promotes adhesion and stiction-related failure; low humidity promotes increased friction between contacting surfaces</td>
</tr>
<tr>
<td>Mechanical Failure</td>
<td>Size effects result from interaction of dislocations with grain boundaries, free surfaces, and interfaces. Vacancy nucleation occurs due to long-term fatigue cycling. Mechanical stress and creep occur due to large temperature variation. Spalling, ductile and brittle fracture and delamination occur during shock loading</td>
</tr>
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</table>

Table 2.1: Failure mechanisms in contacting RF MEMS
MEMS switch are summarized in Table 2.1. Dielectric charging is caused by trapped charges inside the thin dielectric layer and leads to uncontrollable changes of the actuation voltage versus time, and eventually, complete device failure. Contact area damage and wear leads to contact resistance degradation even for relatively low power levels. It is often manifested as contact resistance increase versus time that renders the switch unusable. MEMS switches are very sensitive to environmental contaminants and humidity. While hermetic on-wafer packages have been developed (e.g. Ref. 7), the ideal environment around the switch is still unknown. Mechanical failure mechanisms are tied to reductions in the physical size of the device, resulting in an interaction of microstructure with interfaces and free surfaces. Mechanical stress and creep development are important at very high or very low temperatures (e.g. operation at 460°C and/or temperature swings of -180 to +120°C), but virtually no studies exist today on this issue. Under conditions of shock loading, mechanisms related to materials microstructure, such as spalling, ductile and brittle fracture and delamination, become important.

2.2 Prediction Goals
In developing prediction goals for the Center, it is useful to understand the state-of-the-art in lifetime measurements for the class of capacitive contacting RF-MEMS that forms our target system. Fig. 2.2 shows published data on lifetime (cycles to failure) versus activation voltage for this class of MEMS for a number of university and industrial switches. Though these switches are ostensibly of the same (or very similar) designs, measured lifetimes vary by 1-2 orders of magnitude or more. The sources of this variation are not well understood, and may lie in the fabrication processes and differences in testing protocols, among others. A simulation capability which can predict mean device lifetime to within an order of magnitude of...
the experimental mean lifetime is not available today, and forms one of the central goals of this Center.

The specific metrics for measurement of lifetime are related to the pull-in and release voltages for the switch. Fig. 2.3 (a) shows the variation of the gap height $g$ with applied bias in an RF-MEMS switch. When a bias $V_{\text{bias}}$ is applied to the metal membrane (Fig. 2.3 (b)), the gap height remains nearly constant until the pull-in voltage, $V_{\text{pull-in}}$, is reached. At this point, the membrane snaps shut, closing the switch. Since the electro-static force varies as the inverse of the gap squared, decreasing the applied bias keeps the contact closed until the bias has fallen below the pull-out voltage $V_{\text{pull-out}}$. Below this value, the membrane is released. Dielectric charging, a critical failure mechanism for this type of device, causes the pull-in and pull-out voltages to drift with time.\(^4\) When the dielectric is held at a positive voltage $V(t)$ with respect to the membrane negative charges accumulate in the dielectric, reducing both the pull-in and pull-out voltages with time, as seen in Figs. 2.3(c). When the pull-out voltage falls below the minimum voltage applied by the pulse, the result is electrostatically-induced stiction. We define device failure as an unacceptably low value of the pull-out voltage, $V_{\text{pull-out}} = 0$ for the case shown in Fig. 2.3(c).

The role of contact and impact on device failure is poorly understood. If device failure due to dielectric charging is related primarily to the total charge accumulated with time, then the number of cycles to failure should be related only to the total contact time between the membrane and the dielectric, and not to whether there is periodic impact. At present, there is no clear consensus on whether contact mechanics are central to failure, though anecdotal evidence exists. An important goal of the center is to delineate the effects of contact and impact on device failure. To tease out these effects, we propose to conduct experiments and simulations under sustained contact, i.e., under conditions in which the membrane is activated by a voltage greater than the pull-in voltage, and is held in contact with the dielectric over extended lengths of time (i.e., contact without impact). The pull-out and pull-in voltages are then measured periodically. If the drift in these quantities mirrors that for the periodic contact case, dielectric charging would be established as scaling primarily with the total time of contact between the metal and the dielectric; else, the dynamics of contact and impact will have been established as central to failure.

Another metric for device failure is the ability of the switch to maintain the gap $g$ at constant voltage. Given an applied voltage, the gap is found to decrease with time due to creep and dielectric charging (Fig. 2.4). A measure of the predictive capability of PRISM codes is their ability to predict the gap versus time behavior of RF MEMS switches.

However, even with petascale simulation capabilities, it is not possible to perform simulations of billions or trillions of cycles. Thus, our goal is to predict the curves in Fig. 2.3(c) under accelerated testing scenarios. Thus, the PRISM center has three 5-year prediction goals:

- The first goal is to predict the mean failure lifetime for the case of periodic contact, as shown in Fig. 2.3(c), to within one order of magnitude of switch lifetime measurements to be made at Purdue. This will be achieved by making multi-cycle predictions under accelerated testing scenarios at higher-than-normal voltages.

- The second goal of the center is to predict mean failure lifetime for the case of sustained contact. This will be achieved by making sustained contact simulations under accelerated testing conditions at higher-than-normal voltages. Pull-in and pull-out voltages are to be predicted within 20% of the experimental mean.

![Fig. 2.4: Variation of gap versus time at fixed voltage.](image)
- The third goal is to predict critical slopes in the gap-versus-time curves at fixed voltage, as shown in Fig. 2.4. The goal is to make predictions to within 20% of experimental values.

2.3 Center Organization
The organization of PRISM is driven by the Center’s prediction goals, and is shown in Fig. 2.5. Prof. Jayathi Y. Murthy, Robert V. Adams Professor of Mechanical Engineering, directs the center. Prof. Murthy reports to Dr. Alan Rebar, Executive Director of Discovery Park and Senior Associate Vice President for Research. She is assisted by three Associate Directors, Professors Anil Bajaj, Weinong Chen and Ananth Grama. Mr. Matt Potrawski serves as the Managing Director and oversees the day-to-day running of the Center. Overall coordination of the software development is the responsibility of the Chief Software Architect, Dr. Michael McLennan, while Prof. Alina Alexeenko oversees our Education and Outreach efforts. PRISM operations are overseen by a Leadership Council composed of the Director and Associate Directors, the Managing Director and the Chief Software Architect. An External Advisory Board consisting of stakeholders in the MEMS manufacturing community, computational and design software firms, representatives of defense industries with MEMS applications, as well as University leaders, guide the overall directions of the Center. The current members of the Advisory Board are listed in Table 2.2.

PRISM research is conducted under three science thrusts. Thrust 1, Contact Physics, is coordinated by Prof. Ashraf Alam. Thrust 2, Multiscale Modeling of MEMS Response, is coordinated by Prof. Marisol Koslowski, and Thrust 3: Multiscale Modeling of Aerodynamic Damping, is led by Prof. Alina Alexeenko. The activities of these groups are supported by two cross-cutting research thrusts, Computational Science and Engineering, led by Prof. Sanjay Mathur, and Uncertainty Quantification Science, led by Prof. Dongbin Xiu. Table 2.3 shows the composition of the different thrusts, team roles and the expertise of individual members.

The uncertainty quantification activities of the Center are central to the Center mission and are overseen by a UQ Coordinating Group consisting of all the major thrust leads and software leads, and

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<thead>
<tr>
<th><strong>Affiliation</strong></th>
<th><strong>Expertise</strong></th>
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<tbody>
<tr>
<td>Prof. Andreas Cangellaris (Chair)</td>
<td>Electrical and Computer Engineering, University of Illinois, Urbana Champaign</td>
</tr>
<tr>
<td>Dr. Jim Allen</td>
<td>Sandia National Laboratories</td>
</tr>
<tr>
<td>Dr. M.S. Anand</td>
<td>Rolls Royce</td>
</tr>
<tr>
<td>Prof. Bharat Bhushan</td>
<td>Mechanical Engineering, Ohio State University</td>
</tr>
<tr>
<td>Dr. Marco Brunelli</td>
<td>Siemens Energy</td>
</tr>
<tr>
<td>Dr. Barry Farmer</td>
<td>AFRL</td>
</tr>
<tr>
<td>Dr. Chuck Goldsmith</td>
<td>MEMtronics Inc.</td>
</tr>
<tr>
<td>Prof. Yogesh Jaluria</td>
<td>Mechanical Engineering, Rutgers</td>
</tr>
<tr>
<td>Dr. Ravi Mahajan</td>
<td>Intel</td>
</tr>
</tbody>
</table>

Table 2.2: PRISM External Advisory Board
chaired by Prof. Murthy. This group meets weekly to discuss, plan and coordinate all UQ-related activities. The Target Simulation Lead, Prof. Ale Strachan, coordinates all activities associated with completing the yearly milestone simulations (see Section 3) on schedule. Dr. Mike McLennan oversees Software Engineering. These groups and individuals perform an integrative function, knitting together the activities of the individual thrusts.
<table>
<thead>
<tr>
<th>Thrust 1: Contact Physics</th>
<th>Affiliation</th>
<th>Expertise</th>
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<tbody>
<tr>
<td>A. Alam (Lead)</td>
<td>Electrical and Computer Engineering, Purdue</td>
<td>Reliability, device physics, coarse-grained modeling</td>
</tr>
<tr>
<td>A. Grama</td>
<td>Computer Science, Purdue</td>
<td>Coarse grain MD, parallel computations with ReaxFF</td>
</tr>
<tr>
<td>D. Peroulis</td>
<td>Electrical and Computer Engineering, Purdue</td>
<td>MEMS physics and experiments</td>
</tr>
<tr>
<td>A. Raman</td>
<td>Mechanical Engineering, Purdue</td>
<td>Stiction/adhesion physics and experiments</td>
</tr>
<tr>
<td>A. Strachan</td>
<td>Materials Science and Engineering, Purdue</td>
<td>Atomic-level modeling of contact physics</td>
</tr>
<tr>
<td>H. Kim</td>
<td>Materials Science and Engineering, Purdue</td>
<td>Atomic-level modeling of contact physics</td>
</tr>
</tbody>
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<table>
<thead>
<tr>
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<th>Affiliation</th>
<th>Expertise</th>
</tr>
</thead>
<tbody>
<tr>
<td>M. Koslowksi (Lead)</td>
<td>Mechanical Engineering, Purdue</td>
<td>Multiscale materials modeling</td>
</tr>
<tr>
<td>A. Alam</td>
<td>Electrical and Computer Engineering, Purdue</td>
<td>Electrical transport theory and modeling</td>
</tr>
<tr>
<td>N. Alur</td>
<td>Mechanical Science and Engineering, UIUC</td>
<td>Multiscale/multiphysics simulation of MEMS</td>
</tr>
<tr>
<td>A. Bajaj</td>
<td>Mechanical Engineering, Purdue</td>
<td>Non-linear dynamics, reduced-order modeling</td>
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<tr>
<td>T. Fisher</td>
<td>Mechanical Engineering, Purdue</td>
<td>Sub-micron heat transfer modeling and experiments</td>
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<tr>
<td>J. Murthy</td>
<td>Mechanical Engineering, Purdue</td>
<td>Sub-micron heat transfer modeling, numerics</td>
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<td>A. Strachan</td>
<td>Materials Science and Engineering, Purdue</td>
<td>Atomic-level materials modeling</td>
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<tr>
<td>D. Sulsky</td>
<td>Mathematics, University of New Mexico</td>
<td>Material point method, computational mechanics</td>
</tr>
<tr>
<td>P. Wallstedt</td>
<td>Mathematics, University of New Mexico</td>
<td>Material point method, computational mechanics</td>
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<tr>
<td>G. Venturini</td>
<td>Materials Science and Engineering, Purdue</td>
<td>Coarse-grained modeling</td>
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<tr>
<th>Thrust 3: Multiscale Models for Aerodynamic Damping</th>
<th>Affiliation</th>
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<tbody>
<tr>
<td>A. Alexeenko (Lead)</td>
<td>Aeronautics and Astronautics Engg., Purdue</td>
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<td>Physics of aerodynamic damping and non-linear dynamics</td>
</tr>
<tr>
<td>L. Sun</td>
<td>Mechanical Engineering, Purdue</td>
<td>Computational fluid dynamics</td>
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<tr>
<td>D. Xiu (Lead)</td>
<td>Mathematics, Purdue</td>
<td>Generalized polynomial chaos</td>
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<tr>
<td>N. Alur</td>
<td>Mechanical Science and Engineering, UIUC</td>
<td>Stochastic methods for multiscale/multiphysics systems</td>
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<td>S. Mahadevan</td>
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<td>Uncertainty quantification, Bayesian methods</td>
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<tr>
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<td>S. Mathur</td>
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<td>FVM, IBM implementation, MEMOSA integration</td>
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<tr>
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<tr>
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<tr>
<td>P. Wallstedt</td>
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<th>UQ Coordinating Group</th>
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<tr>
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<tr>
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<tr>
<td>A. Alexeenko</td>
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<td>Thrust 2 models</td>
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<td>M. Koslowksi</td>
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<tr>
<td>A. Mathur</td>
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<tr>
<td>A. Strachan</td>
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</tr>
<tr>
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<td>G. Venturini</td>
<td>Materials Science and Engineering, Purdue</td>
<td>Uncertainty quantification</td>
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Table 2.3: Team composition, team roles and expertise
2.3.1 Thrust 1: Contact Physics
The focus of this thrust is failure mechanisms directly associated with metal-dielectric contact, including dielectric charging, current channeling, contact-area evolution and damage, and the influence of environmental factors such as humidity. A significant focus of the center is the atomistic resolution of adhesion and stiction phenomena, and their influence on macroscale physics. To address dielectric charging, physics-based models are developed to model the capture of injected electrons by new traps, the spatial and temporal distortion of the electric field as a result, and finally, the dynamic feedback due to the resulting spatial inhomogeneities.\textsuperscript{12} Models capturing these physics are incorporated in our finite volume framework. Current channeling and contact area evolution occur as dielectric and metal make non-uniform contact because of surface roughness, causing preferred current pathways to form; these evolve dynamically as repeated contact modifies the surface morphology and as preferred current pathways evolve in a dynamic manner.\textsuperscript{13,14,15} These physics are captured at the microscale through the use of large-scale non-equilibrium molecular dynamics (MD) simulations describing metal-dielectric contact under periodic impact.

2.3.2 Thrust 2: Multiscale Modeling of MEMS Response
The focus of this thrust is to develop an integrated electro-thermo-mechanical model for the structural behavior and dynamic response of the metallic membrane and auxiliary structures. Though classical theories are expected to be valid for the most part, attempts to investigate thinner membranes or to understand the long-term influence of microstructure on macroscopic behavior must contend with the sub-micron effects. When the critical dimension of the device falls into the sub-micron range, material properties can no longer be approximated by bulk values, surface effects become dominant, and material inhomogeneities such as defects and dislocations can play an important role. Material constitutive relations are being developed based on atomic-level dynamics, and on meso-scale phase field micromechanical models (PFMM). Dislocations and defects are described by continuum fields and work is underway to integrate them seamlessly in macroscale material descriptions.\textsuperscript{16,17} Key components of our approach are: (i) grain texture and orientation in Ni membranes, including a dislocation-based model of polycrystalline plasticity, (ii) accounting for residual stress and defect concentrations (vacancies and dislocations) due to the manufacturing process, (iii) single and polycrystalline plasticity integrating finite elastic and plastic deformation induced by micro-defect formation; dislocations are individually tracked and naturally take into account size effects in plastic deformation, and (iv) changes in contact area topology and in the material mechanical properties due to accumulation of defects.

2.3.3 Multiscale Modeling of Aerodynamic Damping
The primary focus of this thrust is to resolve the transient aerodynamic damping force that results from membrane motion in the air/N\textsubscript{2} atmosphere in the RF MEMS device. A critical aspect is the transition in flow regimes as the gap between the membrane and the contact pad closes and opens. Flow rarefaction affects aerodynamic damping at small gap sizes, and can be characterized by the Knudsen number, Kn = \lambda/g, the ratio of the molecular mean free path \lambda to the gap size g. The Navier-Stokes equations describe aerodynamic damping of microbeams and membranes at small Kn (<0.01).\textsuperscript{18,19,20} The Navier-Stokes equations augmented by slip/jump conditions to account for tangential slip and temperature jumps, extend the applicability of the continuum model up to Kn=0.1.\textsuperscript{12} For high Kn (>0.1) the deterministic ellipsoidal-statistical Bhatnager-Gross-Krook (ES-BGK) model\textsuperscript{22} has been found to agree with experiments\textsuperscript{23} for a wide range of rarefaction. In this thrust, we adopt a deterministic approach combining
the Navier-Stokes and the Boltzmann equations and switching between the two as the switch gap closes. The continuum Navier-Stokes equations are used for the flow regions where the local Knudsen number (based on local gradients of macro-parameters such as pressure and velocity) is below a breakdown value. Fully-kinetic Boltzmann simulation using an ES-BGK relaxation time approximation is carried out in non-continuum regions which will be automatically detected. Work is underway to integrate the two approaches in our unstructured solution-adaptive finite volume solver.

2.3.4 Computational Science and Engineering
This activity provides a strong backbone of computational and algorithmic expertise in the petascale simulation of molecular systems, and in the development and deployment of parallel linear solvers. An adaptive library of linear solvers is being developed to serve Center simulation activities and to ensure performance portability across different petascale architectures. It is likely that both direct and iterative solvers will be necessary. A variety of parallel direct solvers, for example, Harwell Subroutine Library solvers such as MA48 or MA5725, Berkeley's SuperLU26, CERFACS' MUMPS26, or Intel's MKL solver PARDISO27, are available. These algorithms have different reordering strategies during the factorization stage and exhibit different computation/communication time ratios, depending on the computing platform. If a reordering scheme produces a banded system that is sparse within the band, these solvers can be used as kernels in the SPIKE algorithm,28 thus enhancing overall parallel performance on a variety of parallel architectures. The library also provides preconditioned iterative solvers using Krylov subspace methods as the outer-most iteration. When the coefficient matrix is available explicitly, efficient preconditioning schemes will be developed by extracting banded systems using reordering schemes to minimize the system's bandwidth.29,30,31 These schemes bring most of the largest matrix elements into a relatively narrow band centered around the main diagonal. Such central bands are then used as pre-conditioners, and systems involving them are solved using members of the SPIKE family of algorithms, which achieve high performance on parallel computing platforms.

2.3.5 Uncertainty Quantification Science
During the last year, we have developed a Bayesian network framework as the central organizing principle to integrate multiple sources of uncertainty and error, and for effective uncertainty quantification in MEMS simulation.32,33 Uncertainty quantification in PRISM switch simulations involves accounting for multiple length and time scales, and involving a variety of physics. Both simulations and experiments are of varying levels of fidelity, and in many instances, available experimental data may not be for the same switch design. In some instances, the uncertainty in inputs and outputs is well-characterized, whereas in others, expert opinion is all that is available. The methodology integrates the contributions of input variability, data uncertainty (experimental and other sources), and model uncertainty and error, at multiple levels of the system hierarchy. The components of this effort include model calibration, model validation, error and uncertainty quantification, confidence assessment in system-level prediction, and sensitivity analysis.

A typical network representation of the PRISM switch response is shown in Fig. 2.6. Integral to the Bayesian network approach is efficient representations of the input-output response of the models (yellow) in Fig. 2.6. PRISM adopts a hierarchical approach, culling unimportant variables for each sub-model. Approximate techniques such as linear sensitivity are used to perform this culling, and PRISM codes employ automatic code differentiation to provide linear sensitivity coefficients. Generalized polynomial chaos (gPC) is a central tool being used in PRISM34,35,36,37,38 to propagate uncertainty from inputs to outputs at each model node in Fig. 2.6. Though gPC traditionally employs the Galerkin method, a newly-developed collocation scheme39 used in conjunction with sparse-grid representations of the
random space is especially powerful for more complicated governing equations. Adaptive techniques which cluster collocation points in random space depending on the local gradients of the output variable are also being developed.\(^\text{40}\) Galerkin gPC methods are intrusive, and existing codes must be significantly modified to admit stochastic analysis. This is difficult to do with legacy software. Discrete Galerkin approaches to gPC\(^\text{41}\) have been developed which exploit operator overloading and templating to achieve unintrusive implementations of gPC within our MEMOSA software suite (see below).

2.4 Software Engineering and Solver Integration

PRISM software is integrated under a single environment called MEMOSA (MEMS Overall Simulation Administrator) to enable full-system simulation. A conceptual layout of the MEMOSA simulation environment is shown in Fig. 2.7, and consists of a pre-processing suite of CAD geometry and mesh generation software, a solver suite consisting of finite volume, material point, molecular dynamics, and mesoscale micromechanical modeling software, and a post-processing suite to enable the parallel visualization of large data sets. Communication between the micro- and macro-scales is accomplished through a compact model database, which is populated by running the microscale solvers offline. The computationally-intensive kernels in MEMOSA are written in a compiled language such as C/C++ or F95 while the driving logic, parameter setting and user interfaces are implemented in Python. Execution of parallel applications is also possible using extensions such as PyMPI. Existing codes are adapted to this paradigm with relatively little effort using tools such as Simplified Wrapper and Interface Generator (SWIG)\(^\text{32}\) that help in creating interpreted language bindings. In this manner, different components can use different languages and programming styles, and legacy and newly-written code can interoperate seamlessly. In addition to providing support for the execution model, MEMOSA also supplies a Subversion repository, a common set of build tools, basic data structures and utilities that are shared by all new software being developed.

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### Team Members

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<thead>
<tr>
<th>Software Engineering</th>
<th>Lead: M. McLennan, RCAC, Purdue</th>
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<td>M. Koslowski, ME, Purdue</td>
<td>F. Saied, RCAC, Purdue</td>
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<td>F. Saied, RCAC, Purdue</td>
<td>D. Sulsky, Math, UNM</td>
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<tr>
<td>B. Yildirim, RCAC, Purdue</td>
<td>M. McLennan, RCAC, Purdue</td>
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Fig. 2.6: Bayes network for simulation of failure lifetime in PRISM switch
2.4.1 Key Software Components
The MEMOSA system consists of the following software components:

- **MEMOSA-FVM**, an unstructured solution-adaptive finite-volume solver,\(^{43,44}\) which forms the computational basis with which to address fluid flow, heat transfer, electro-statics, rarefied gas dynamics and charge and species transport in MEMOSA.

- **MEMOSA-MPM**, a solver based on the material point method (MPM), which forms the basis for the computation of structural deformation and for the incorporation of micromechanical materials models.\(^{45}\) MEMOSA-MPM and MEMOSA-FVM are coupled using the immersed boundary method (IBM).\(^{46}\)

- **MEMOSA-PFMM**, a 3D solver for computing dislocation dynamics for the development of micromechanical materials models.

- **LAMMPS**, a molecular dynamics solver developed at Sandia National Laboratories,\(^{47}\) designed to perform very efficiently on parallel architectures, and capable of addressing a large variety of atomic, metallic, granular and coarse-grained systems. LAMMPS is used for atomistic contact simulations in PRISM.

In addition, **PuReMD**, a molecular dynamics solver using reactive force fields, is being developed for the computation of surface reactions at contacting surfaces.\(^{48}\) A more detailed description of the solver is given in Section 5.

2.5 Coarse-Grained Solver for System Simulation
We have developed a coarse grained model which accounts for the non-idealities like dielectric charging, creep and squeeze film damping in a simple and coherent way that can be adapted to interpret experiments and to obtain a broad picture of the most important determinants of system performance quickly. The system considered is shown schematically in Fig. 2.8, and consists of a thin elastic membrane held rigidly between two supports. It is actuated electrostatically by an electrode of width \(2a\), and in its undeformed state, is situated at gap height \(h\) above it. The motion of the membrane is damped by the presence of a gas. Furthermore, dielectric charging in the substrate is also accounted for, using spatially-integrated charges in the dielectric obtained using the dielectric charging model described in previous sections. A table-lookup procedure is used as a function of the applied voltage to obtain the integrated charge, which modifies the applied electrostatic force.

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Fig. 2.7: A schematic showing the principal components of MEMOSA
The equation governing the transverse membrane deformation $w(x)$ is given by the Euler-Bernoulli beam equation:

$$\rho_l \ddot{w} - \frac{EI}{1 - \nu^2} \frac{d^4 w}{dx^4} - b \frac{\partial w}{\partial t} + F_{\text{elec}} = 0$$

where $\rho_l$ is the membrane density, $E$ its Young’s modulus, $I$ its moment of inertia, $\nu$ the Poisson ratio, $b$ the fluid damping coefficient and $F_{\text{elec}}$ the electrostatic force. The damping coefficient $b$ is taken from a correlation developed by Prof. Alina Alexeenko’s group using the ES-BGK model, and is applicable to a wide range of Knudsen numbers. \cite{49}

$$b = \frac{A \left( \frac{W}{h} \right)^c t}{1 + B \left( \frac{W}{h} \right)^d \left( \frac{\lambda}{W} \right)^e}$$

Here, $A$, $B$, $c$, $d$ and $e$ are constants in the curve fit from Ref. 49, $W$ is the width of the membrane, $t$ its thickness, and $\lambda$ the gas mean free path. To model contact between the membrane and the dielectric, a multiscale contact model, described in Section 8, has been incorporated in Year 3. A model for creep relaxation, described in Section 5, has been incorporated as well. The coarse-grained model has been used to compute cycles-to-failure and its sensitivity to input variables, as well as for the propagation of input uncertainties through a multiscale system simulation.

### 2.6 Verification and Validation

PRISM’s verification and validation procedures mirror those that have been developed by NNSA laboratories. \cite{50,51} The overall verification, validation and uncertainty quantification procedure used in PRISM is that defined in Ref. 52; the specific steps are shown in Fig. 2.9. In keeping with these procedures, a phenomena identification and ranking table (PIRT) is developed which identifies all critical components of the physics models, numerical techniques and software implementation and ranks their importance \textit{vis a vis} the simulation goal. Based on the PIRT, a verification test suite (VERTS) and a validation test suite (VALTS) are developed. Because of the sheer complexity of the phenomena being modeled, a 3-tier system is adopted for both VERTS and VALTS. Verification and validation tests target single-physics phenomena first, building to phenomena involving two interacting phenomena, and finally addressing multiple coupled phenomena at the system-level.

Once the PIRT, VERTS and VALTS are determined, code verification is performed. This includes verification of numerical algorithms through comparisons with exact solutions, manufactured solutions, and tests for symmetry and iterative convergence, among others. Asymptotic convergence tests are also performed to establish that the code is yielding the expected solution order. Software quality assurance procedures such as configuration management, nightly build and test, and regression testing have been put in place. Once a verified code is available, the focus now shifts to the simulation of interest. Solution verification is performed to establish mesh independence, and to establish discretization error through \textit{posteriori} error estimation procedures such as Richardson’s extrapolation.
Once this is done, the validation procedure begins. For any given model node in the Bayes network in Fig. 2.6, sensitivity analysis and effect screening are first performed to identify the most important input variables; this may be done either using a design of experiments approach, or more recently, using lower-degree cubature collocation techniques, among others. A meta-model may then be constructed if necessary. Uncertainty propagation techniques are then used, either on the meta-model, or on the original model, to propagate uncertainties in inputs to the outputs. At PRISM, the current focus is to use the lower-degree cubatures in Ref. 54 in conjunction with collocation to propagate uncertainty, though other techniques are also being investigated. During the last year, Bayesian validation approaches have been investigated, using the concept of the Bayes factor, as described in Ref. 55.
3. **PREDICTION GOALS AND SIMULATION ROADMAP**

The 5-year simulation goals for the Center are shown in Fig. 3.1, and are described below.

- **Year 1**: In Year 1, there are two focus areas. The first focus is on the simulation of fluid-structure interaction in MEMS structures in the continuum regime for small displacements, that is, without metal-dielectric contact, and the prediction of damping coefficients as a function of system Knudsen number, with comparisons to experiments performed at Sandia and at Purdue. The second focus is on performing metal-metal and metal dielectric simulations of atomistic contact with the potentials available in LAMMPS to determine the pull-out force and contact area evolution.

- **Year 2**: In Year 2, there are four focus areas. The first is the prediction of fluid damping for the PRISM device, as opposed to the simple cantilever structures considered in Year 1. Furthermore,
the slip regime for fluid damping is to be addressed. The second is the extension of the fluid-structure interaction computations to include electrostatic forces, and thus to predict membrane deformation as a function of applied voltage. The third focus is to simulate dielectric charging for a static metal-insulator-metal (MIM) capacitor with the objective of predicting trap charge density as a function of time, voltage and voltage cycling. The last focus area is the computation of metal-dielectric contact through the use of improved potentials to predict pull-out force and contact area evolution, and to provide data to the development of micromechanical and dielectric charging models.

- **Year 3**: Year 3 simulations will address device simulations with large deformations and metal-dielectric contact for single-contact events. Dielectric charging computations will be initiated for the case of sustained contact. Contact modeling at the meso- and atomistic scales will be integrated to include plasticity effects. The fluid damping model will be extended to the rarefied regime through the use of the ES-BGK formalism. The development of models for creep will be initiated.

- **Year 4**: In the fourth year, simulations addressing the three main PRISM goals will be initiated. These will include PRISM device simulations under periodic and sustained contact under accelerated testing conditions, and PRISM device gap-versus-time simulations to simulate creep effects. Predictions will be compared to device life-time measurements made at Purdue. These simulations are estimated to be of long duration, particularly when conducted under a UQ framework. They are expected to extend into Year 5.

- **Year 5**: In the fifth and final year of the center, simulations initiated in Year 4 will be completed, and uncertainty quantification in these simulations completed.
4. SUMMARY OF YEAR 3 MILESTONES AND ACCOMPLISHMENTS

We summarize below the milestones that have been met during Year 3.

**Milestone 1: Structural Response Simulations.** Here, the focus is on the prediction of the structural response of the PRISM device under the influence of fluidic damping and electrostatic actuation for two cases: (i) membrane pull-in under the action of electrostatic force and fluid damping but with no impact or contact, and (ii) the dynamical membrane pull-in and pull-out response under the action of electrostatics and fluid damping, and with contact and impact with the pull-down electrode. For the first of these simulations, good agreement with measured experimental data has been obtained, including a quantification of uncertainty. For the second, deterministic simulations of multi-cycle contact have been completed; measurements of the contact dynamics are underway, as well as uncertainty quantification of these simulations.

**Milestone 2: Dielectric Charging Simulation Under Sustained Contact.** Under this milestone, the focus is on the predictive simulation of charging in a metal-insulator-metal (MIM) capacitor in which metal and insulator are in contact, but there is no periodic impact. A new multi-trap depth dielectric charging model has been developed and integrates atomistic descriptions of defect levels with a mesoscale model for the charging the silicon nitride dielectric. The model has been calibrated to charging data on the MIM capacitor. Simulations of charging in the MIM capacitor have been performed, and identify the trap depth and barrier height as the primary determinants of uncertainty in dielectric charging predictions. Computations are underway to integrate the model in multi-cycle contact simulations.

**Milestone 3: Uncertainty Quantification of Membrane Creep Predictions.** The focus of the Year 3 work is the prediction of membrane creep for non-contacting structures. We have focused on the problem of Ni membrane deformation under the influence of a fixed applied voltage, and the prediction of the change of gap with time. A Coble creep model for second-stage creep has been developed, and used in MEMOSA to predict the evolution of gap versus time for a frogleg varactor for which long-term creep data have been measured at Purdue. A Bayesian network approach is adopted, and Bayesian calibration of creep constants and subsequent analysis indicate that model-form error, possibly resulting from the neglect of residual stress, is significant. Simulations are underway on the PRISM MEMS structure, and long-term experimental measurements on the same structure are currently being completed.

**Milestone 4: Uncertainty Quantification of Coarse-Grained System Simulation.** We developed a coarse-grained solver suitable for system simulation based on the work performed in Year 2. In Year 3, lifetime predictions using the model were performed, coupling elastic membrane response, electrostatics, fluid damping and dielectric charging, and the major sensitivities of the time-to-failure to system inputs were identified. Furthermore, the coarse-grained model was used to develop and evaluate multi-scale coupling and uncertainty propagation during a single-event contact simulation of dynamic pull-in and pull-out and for long-term creep predictions. Furthermore, the model has been used to investigate near-contact damping, and to provide verification in the high aspect ratio limit for MEMOSA-FVM structural computations. These coarse-grained simulations lay the ground-work for substituting the coarse-grained model with a full-system MEMOSA simulation in Year 4, and establish the essential framework for system-level uncertainty quantification.

In addition to meeting these milestones, significant advances have been made in developing the experimental, numerical and software infrastructure. These include:

- **Experimental Data for Validation.** Damping factors for a range of pressures from 10 Pa to atmospheric were measured for the PRISM device for multiple replicates of the same device, as well as for multiple devices. Characterization of the input geometry (membrane length, thickness, gap) was also performed. Experiments to characterize the long-term creep/viscoelastic behavior...
of the nickel membrane in the PRISM device were also conducted. A new generation of PRISM switches, Generation 5, were fabricated and pull-in measurements performed.

- **Improvements to Physical Models for Membrane Deformation.** Significant improvements to the materials models in MEMOSA have been made in Year 3. A plate element model has been developed in MEMOSA-FVM to enable the efficient and accurate simulation of membrane deformation in high aspect ratio membranes, and coupled to the immersed boundary method; extensions for creep have also been developed. Furthermore, an *anisotropic elasticity* model as well as a *J2 plasticity* model with linear isotropic hardening have been developed and implemented in MEMOSA-MPM to model membrane deformation.

- **ES-BGK Model for Rarified Gas Dynamics in MEMOSA-FVM.** Implementation of the ellipsoidal-statistical Bhatnagar Gross Krook (ES-BGK) model for rarefied gas dynamics has completed in MEMOSA-FVM and verification tests have been performed.

- **Advances in Uncertainty Propagation Methodologies.** The *adaptive collocation scheme* developed in Year 2 to address collocation gPC in the presence of steep gradients and discontinuities in random space was enhanced and integrated in MEMOSA.

Furthermore, a comprehensive educational program has been established, including workshops, a seminar series, additions to the Computational Science and Engineering program, and a student internship program at the national laboratories. The MEMShub web portal has been enhanced and is used to disseminate research, software, experimental data and pedagogical materials to the MEMS community.

In the next few sections, we amplify on these accomplishments. In Section 5, results of the milestone simulations undertaken in Year 3 are described. In Section 6, the experimental program undertaken in Year 3 is described. Section 7 describes advances in the development of uncertainty quantification methodologies. Section 8 describes the advances made in the individual science thrusts and cross-cutting thrusts. Section 9 describes enhancements made to the MEMOSA software system, to the underlying numerical methods, and to parallel scaling. Educational and outreach accomplishments are described in Section 10.
5. MILESTONE SIMULATIONS

5.1 Uncertainty Quantification of Static and Dynamic Pull-In

During Year 3, gap-versus-voltage and pull-in simulations of PRISM Generation 2 devices were conducted using MEMOSA. PRISM Generation 2 was fabricated during September 2009- March 2010, and measurements of gap versus voltage and pull-in voltage were made. Gen 2 consists of a variety of devices of the same nominal design as in Fig. 2.1, but with varying membrane lengths, widths, thicknesses and gaps. Of these, we focused on simulating device #2-3D, whose specifications are given in Table 5.1. The computational domain and simulation parameters are shown in Fig. 5.1.

Fig. 5.2 shows our prediction of gap versus voltage and a comparison with experimental measurements for device 2-3D. The simulations were performed assuming no residual stress, and assuming the bulk value for Young’s modulus of nickel. Furthermore, the simulations were performed using a static formulation, that is, inertial terms were neglected. The comparison of the predictions and experiments is reasonably good for voltages lower than pull-in, with a COV of about 18%. The experimental value of pull-in is found to be 232.5V ±2.5 V. The predicted static pull-in value is 237.5±2.5 V. This is in keeping with the fact that Gen 2 devices have tensile residual stress that is unaccounted for in the simulations. Thus, the simulated membrane is in effect more stiff than the real membrane, and would be expected to pull in at a higher voltage. Transient simulations of pull-in were also performed, and the predicted dynamic pull-in value is found to be 227.5V±2.5 V. Furthermore, the computed dynamic pull-in voltage is about 10% smaller than the computed static pull-in voltage as a result of inertial forces aiding pull-in. The experiments themselves are performed sequentially, with the voltage being stepped up from the last deformed position, whereas both static and dynamic simulations are performed starting from the undeformed position. The experimentally-measured value would thus be expected to lie between the computed static and dynamic pull-in values.

Uncertainty quantification of dynamic pull-in was also performed during the last year. Figure 5.3 shows the uncertainty in the maximum deflection versus time for the PRISM Gen 2 device for two different activation voltages, 190V and 230V, using a third-order PC expansion with uncertain length, gap, thickness and effective Young’s modulus. The uncertainty in the prediction increases with time as some devices tend towards pull-in while others do not; again, the primary determinants of uncertainty are

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Boundary conditions
- No-slip walls with zero potential gradient on external boundaries
- Membrane at 0 V; 3 electrodes at applied voltage

Simulation Parameters
Nominal domain size = 600μm x 21μm x 400μm
Nominal mesh size = 880K+250K (structure+fluid)
Time step = 0.01 μs
Discretization error = 0.948%
Time-step error = 0.06%
Domain size error = 0.0093%

Fig. 5.1: Computational domain and simulation parameters for pull-in simulation.
geometric parameters, as shown in Fig. 5.4. Figure 5.5 shows the PDF of static pull-in voltage. Though the input PDFs are symmetric (Gaussian), the pull-in voltage exhibits a mild asymmetry towards smaller pull-in voltages, and the standard deviation is over 14% of the mean pull-in voltage. Furthermore, the spread in pull-in voltage implies that if the population of devices were activated at the mean pull-in voltage, a significant population would not pull in, while the rest would be over-actuated.

Table 5.1: Input parameters for pull-in simulations.
Fig. 5.2: Maximum displacement versus voltage for device #2-3D.

Experimental uncertainties:
±100 nm for displacement
±1 millivolt for voltage
±2.5 volts for pull-in
Simulation uncertainty:
±0.948%
±2.5 volts for pull-in

Computed static pull-in = 237.5 V ±2.5 volts
Computed dynamic pull-in = 227.5 V ±2.5 volts
Measured pull-in = 232.5 V ±2.5 volts

Fig. 5.3: Uncertainty in maximum displacement versus time for PRISM Gen 2 pull-in.

RMS error = 1.13×10^{-7} m
RMSE/mean = 0.264 overall
= 0.18 <215 volts

Mean=1.15 μm
SD=0.174 μm
COV=0.16

Mean=0.622 μm
SD=0.0995 μm
COV=0.16
Fig. 5.4: PDFs of maximum membrane deflection at $t=2.29$ microseconds at an activation voltage of 250 V. Shown above are PDFs of maximum deflection with all input parameters varying, as well as with each parameter varying while the others are held at their mean values. The greatest contributors to deflection uncertainty are seen to be uncertainties in gap and thickness.

Fig. 5.5: PDF of static pull-in voltage for PRISM Gen 2 device.
5.2 Fluid Damping Predictions in PRISM Device

Simulations of squeeze film damping in the PRISM device were carried out during Year 3. A schematic of the device and its nominal dimensions are shown in Fig. 5.6. Table 5.2 shows the input uncertainties assumed for predictive simulations. Experimental measurements of ringdown were performed by exciting the beam electrostatically, as shown in Fig. 5.7 and measuring the response envelope. Seven devices from PRISM’s Generation 2 were measured, with five replicates for each device. A large range of pressures, for 1 mTorr to 500 Torr, was considered. Experimental histograms of important geometric parameters, such as membrane thickness, gap height and the measured natural frequency of the membrane, are shown in Fig. 5.8, along with histograms of the measured damping coefficient for 4 pressures. Though measurements of damping coefficient are available for pressures ranging from near-continuum to (low Knudsen number) to rarefied (high Knudsen number), computations are restricted to the continuum and slip regimes. The predicted damping coefficient along with uncertainty bars of ±σ are shown in Fig. 5.9. A third-order gPC fit is employed, with inputs as shown in Table 5.2. We see that large uncertainties are engendered in the predicted damping simulations, with a standard deviation of 30% of the mean value, largely as a result in uncertainties in gap and membrane thickness. Furthermore, the predictions overpredict the damping coefficient at lower pressures as a result of the continuum/slip nature of the underlying Navier-Stokes Slip Jump model. In Year 4, the ES-BGK model will be used to compute slip and rarefied-regime damping.

![Schematic of the PRISM device](image)

Fig. 5.6: Description of PRISM device used in fluid damping simulations.

<table>
<thead>
<tr>
<th>Inputs</th>
<th>Nominal value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Membrane Length</td>
<td>395.34 μm</td>
</tr>
<tr>
<td>Membrane Width</td>
<td>120 μm</td>
</tr>
<tr>
<td>Membrane Thickness</td>
<td>3.96 μm</td>
</tr>
<tr>
<td>Gap Height</td>
<td>3.74 μm</td>
</tr>
<tr>
<td>Dielectric thickness</td>
<td>280 nm</td>
</tr>
<tr>
<td>Gas density</td>
<td>Variable</td>
</tr>
<tr>
<td>Gas viscosity</td>
<td>1.8x10^-5 kg/ms;</td>
</tr>
<tr>
<td><strong>Output</strong></td>
<td><strong>Damping Factor</strong></td>
</tr>
</tbody>
</table>

- Nickel membrane
- Si₃N₄ dielectric
- Air environment
- Pressure range 6.65x10⁴-1.8753x10⁶ Pa
- Constant temperature, 300K
- Navier-Stokes Slip Jump model
- 218,752- cell mesh, 250 time-steps
- Estimated discretization error in damping factor is < 2%

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Measurement made at center of beam for ring down data; beam excited electrostatically

- 7 devices
- 16 pressures from 1mT-500T
- 5 replicates of data
- Structural damping calc. from <=300mT

Fig. 5.7: Description of experimental set-up for measuring fluid damping.

Fig. 5.8: Experimental PDFs of (a) device geometry, and (b) measured damping ratio for 4 different pressures, using 7 devices and 5 replicates.
5.2.1 Bayesian Validation of Damping Simulations

The capability of numerical models to accurately predict gas damping coefficient while accounting for epistemic and aleatory uncertainty is key to the failure and reliability analysis of MEMS devices. Four types of methods have been investigated for the validation of a probabilistic MEMS switch damping model, namely classical and Bayesian hypothesis testing, a reliability-based method, and an area metric-based method. Traditional Bayesian hypothesis testing has been extended based on interval hypotheses on distribution parameters and equality hypotheses on probability distributions, in order to validate the predictions from deterministic or probabilistic models. Two types of validation experiments have been considered - well-characterized (known experimental input) and uncharacterized (unknown experimental input). Bayesian hypothesis testing can minimize the risk in model selection by properly choosing the model acceptance threshold $B_{th}$, and its results can be used in model averaging to avoid Type I/II errors.

Bayesian validation of the damping simulations was carried out using the methodology described in Refs. 55 and 58 and based on the experimental measurements of fluid damping described above. Bayesian validation seeks to determine whether model predictions are consistent with experiments, given a defined level of uncertainty. Bayesian hypothesis testing compares two hypothesis, $H_0$ and $H_1$, given data $D$, using Bayes’ Theorem:

$$\frac{\Pr(H_0: \text{model is correct}|D)}{\Pr(H_1: \text{model is incorrect}|D)} = \frac{\Pr(D|H_0: \text{model is correct}) \cdot \Pr(H_0)}{\Pr(D|H_1: \text{model is incorrect}) \cdot \Pr(H_1)}$$

The validation metric is the Bayes factor, $B$, defined as:

$$B = \frac{\Pr(D|H_0: \text{model is correct})}{\Pr(D|H_1: \text{model is incorrect})}$$

Fig. 5.9: Damping ratio predictions and comparison with measurements.
The model of interest is a general polynomial chaos (gPC) surrogate model constructed based on MEMOSA-FVM damping simulations, and validation data were collected from 35 well-characterized experiments under four different gas pressures. The results of Bayesian equality hypothesis testing are shown in Table 5.3 for the purpose of illustration. Based on the performance of the gPC model in these validation tests, it can be concluded that the prediction of the gPC model has better agreement with observation under the middle two values of pressure (28664.31 Pa and 43596.41 Pa), whereas less agreement can be found under the lowest and highest pressure values (18798.45 Pa and 66661.19 Pa).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mean (mm)</th>
<th>Std. Dev (mm)</th>
<th>Comment</th>
<th>Source</th>
<th>Ranking</th>
</tr>
</thead>
<tbody>
<tr>
<td>Membrane length</td>
<td>395.34</td>
<td>3.25</td>
<td>Aleatory; scenario</td>
<td>Exp.</td>
<td>4</td>
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<tr>
<td>Membrane width</td>
<td>120</td>
<td>1.36</td>
<td>Aleatory; scenario</td>
<td>Exp.</td>
<td>5</td>
</tr>
<tr>
<td>Membrane thickness</td>
<td>3.96</td>
<td>0.590</td>
<td>Aleatory; scenario</td>
<td>Exp.</td>
<td>2</td>
</tr>
<tr>
<td>Gap height</td>
<td>3.74</td>
<td>0.270</td>
<td>Aleatory; scenario</td>
<td>Exp.</td>
<td>1</td>
</tr>
<tr>
<td>Gas density</td>
<td>Perfect gas law</td>
<td>--</td>
<td>Constant; model</td>
<td>Lit.</td>
<td>--</td>
</tr>
<tr>
<td>Gas viscosity</td>
<td>1.8x10^4 kg/m/s</td>
<td>--</td>
<td>Constant; model</td>
<td>Lit.</td>
<td>--</td>
</tr>
<tr>
<td>Freq.</td>
<td>9.542x10^3 rad/s</td>
<td>3x10^4 rad/s</td>
<td>Aleatory; model</td>
<td>Exp.</td>
<td>3</td>
</tr>
<tr>
<td>Domain size</td>
<td>280umx100umx50um (1/4 symm)</td>
<td>-</td>
<td>Scenario</td>
<td>Model</td>
<td>&gt;5</td>
</tr>
</tbody>
</table>

Table 5.2: Input uncertainties for fluid damping simulation.

<table>
<thead>
<tr>
<th>Pressure (Pa)</th>
<th>18798.45</th>
<th>28664.31</th>
<th>43596.41</th>
<th>66661.19</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of failures</td>
<td>5</td>
<td>5</td>
<td>3</td>
<td>15</td>
</tr>
<tr>
<td>Failure percentage</td>
<td>14.3%</td>
<td>14.3%</td>
<td>8.6%</td>
<td>42.9%</td>
</tr>
<tr>
<td>Overall Bayes factor (log-scale)</td>
<td>7.4</td>
<td>57.2</td>
<td>72.3</td>
<td>-10.2</td>
</tr>
</tbody>
</table>

Table 5.3: Performance of gPC models in Bayesian equality hypothesis testing (log $B_{th}$ = 1)

5.3 Contact Simulation in MEMOSA

A multiscale contact model was developed in Year 3 for metal-dielectric contact in the presence of surface roughness, and is described in detail in Section 8. Here we describe the results of deterministic simulations that have been performed for pull-in, contact, and pull-out of the PRISM device in the presence of electrostatics and fluid damping.

Fig. 5.10 shows the configuration being simulation. A Generation 5 PRISM device is considered, with dimensions as shown. A plate element model, described in Section 8, is used to model the membrane. The membrane is located in a background mesh on which the electrostatic and fluid flow is computed. The immersed boundary method is used to couple fluid,
structure and electrostatics. A time-dependent voltage pulse, shown in Fig. 5.10, is applied to the membrane, and the dynamical response of the membrane computed. As the membrane approaches contact with the contact pad, the dynamics of contact and bounce are determined by the multiscale contact model. Fig. 5.11 shows the variation of force versus distance resulting from the contact model, and is given by:

\[
f(d) = \frac{H}{6} \frac{1}{d^3} x + \frac{x}{(d - x_0)^3} + B \exp\left[ (d - x_0) \right]
\]

Here, \(d\) is the distance between beam and the substrate. The parameters are given as:

\[
H = 0.23 \times 10^{-20}\; \text{J}; \\
B = 3.529 \times 10^6 \; \text{N/m}^2; \\
x = 0.1127; \\
\gamma = 22.69 \times 10^{-9}\; \text{m}^{-1}; \\
x_{01} = 1.6 \times 10^{-9}\; \text{m}; \\
x_{02} = 1.99 \times 10^{-9}\; \text{m};
\]

In the above equation, the first part of the contact force corresponds to a Van der Waals attractive force and the second part is a repulsive force, as shown in Fig. 5.11 (a). As the membrane approaches the contact pad, the repulsive force increases exponentially. Within a very short distance from the contact pad (~1nm), the repulsive force, the elastic force due to the membrane stiffness and the fluid damping surpass the downward electrostatic force and stops the membrane’s downward motion. Capturing this turnaround requires the use of extremely small time steps, and an adaptive time-stepping scheme is employed to efficiently capture pull-in, contact and pull-out, as shown in Fig. 5.11 (b).

Fig. 5.12 (a) shows the computed dynamical response of the membrane midpoint due to the application of the multi-cycle voltage pulse shown in Fig. 5.10. The effect of fluid damping is quantified in Fig. 5.12. It is seen that fluid damping significantly increases the contact time. This is primarily a result

---

**Computational Details**

- Membrane dimension: 500x120x2 μm
- Background domain dimension: 600x150x10 μm
- Gap: 3 μm
- Dielectric thickness: 200 nm
- Dielectric constant: 7.9
- E: 200 GPa
- Density: 8912 Kg/m³
- Poisson’s ratio: 0.3
- Membrane mesh: 50x10 plate elements
- Background mesh: 60x20x400
- Time step: \(10^{-13} \sim 10^{-8}\) s

---

Fig. 5.10: Configuration for contact simulation
of inverse $d^3$ dependence of the damping coefficient on distance from the contact pad; fluid damping significantly decreases the contact velocity and increases the time required for pull-out.

### 5.4 Dielectric Charging under Sustained Contact

During Year 3, significant effort was devoted to developing and refining a multiscale dielectric charging model and in implementing and testing it in MEMOSA. The dielectric charging model is based on the band diagram shown in Fig. 5.13. By balancing the fluxes due to tunneling, emission, capture and drift, a model for the rate of charge accumulation in the dielectric is developed. The parameters in the model include, among others, the trap depth $\Phi_t$ and the barrier height $\Phi_b$; these parameters are

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computed by calibrating to charging experiments performed using a metal-insulator-metal capacitor, shown in Fig. 5.14. Ab-initio computations of these quantities have also been conducted and yield values in the same range as the experimental calibrations. However, the amorphous nature of silicon nitride leads to defects with a range of energy levels, and points to the need for multiple trap-depth models. The first model developed in Year 3 employed a single value of trap depth and barrier height, and these were used in dielectric charging simulations of the experimental MIM capacitor to determine sensitivity of computed charge accumulation to probabilistic inputs.

Uncertainty quantification of dielectric charging simulations in a metal-insulator-metal (MIM) capacitor was conducted. The details of the simulation are shown in Fig. 5.14. A dielectric of nominal depth 200 nm is charged because of the application of an applied voltage of 100 V as shown. The quantity of interest is the total amount of trapped charge in the domain, given by:

$$Q(t) = \sum_{\text{domain}} \rho_i V_i$$

A list of inputs to the simulation is given in Table 5.4. The primary aleatoric uncertainty is due to the dielectric thickness. The variation of thickness is measured, and is modeled as a uniform distribution with a mean and standard deviation taken from measurements. The other uncertainties in the simulation are due to parametric uncertainties in the dielectric charging model; the ranges of these uncertain parameters and their sources are shown in Table 5.4.

Fig. 5.13: Electronic band diagram for charge injection in metal-insulator-metal (MIM) capacitor.
Our sensitivity analysis reveals that barrier height and trap depth are the two central parameters controlling the uncertainty in the total trapped charges. Figure 5.15 shows the PDF of trapped charges at $t=11.8$ seconds resulting from uncertainty in the dielectric thickness for different combinations of the barrier height and trap depth. Though there is some sensitivity to dielectric thickness, the greatest variation is due to uncertainty in the barrier height and trap depth. Ab-initio simulations to obtain these parameters have been performed and reveal that a single trap depth is not appropriate for this amorphous material. Instead, a distribution of these parameters must be considered. Furthermore, incorporating multiple trap depths also provides better calibration to experimental measurements across a range of temperatures. These details are presented in Section 8.
Fig. 5.15: PDF of trapped charges resulting from aleatoric uncertainty in dielectric thickness for different values of barrier height and trap depth (eV). The dielectric charging model is found to be extremely sensitive to these parameters.
Uncertainty Quantification of Membrane Creep

During Year 3, a model for Coble creep was developed and implemented in MEMOSA-FVM and used for prediction of long-term creep deformation in the frogleg device shown in Fig. 5.16. The frogleg device consists of a plate supported by four legs, as shown in the figure. A constant voltage below the pull-in voltage is applied to the plate. Creep deformation causes the plate to deflect downwards over a period of hundreds of hours. Long-term creep experiments were performed at Purdue using this device. These data provide measurements of gap versus time at an actuation voltage of 20 V.

A large number of constitutive models have been developed for estimating the steady-state creep under different conditions, including power-law creep, Coble creep, Nabarro-Herring creep, dislocation glide, and grain boundary sliding. At any applied stress, the steady-state creep rate can be expressed as:

\[ \dot{\varepsilon}_c \propto \left( \frac{\sigma}{G} \right)^m \]

where \( \dot{\varepsilon}_c \) is the creep strain-rate, \( G \) is the shear modulus, and \( m \) is the creep stress exponent. Different creep mechanisms can be identified with different values of \( m \): diffusion creep is characterized by a linear stress and strain-rate relationship, grain boundary sliding is characterized by \( m = 2 \), and power-law creep is characterized by \( m > 3 \). The creep strain-rate, may be expressed in the form:
where $A_c$ is a material dependent constant. We assume strain-hardening of the form:

$$\dot{\varepsilon}_c = A_c \left( \frac{\sigma}{\sigma_y} \right)^m$$

Here $\varepsilon_{c,\text{eff}}$ is the effective or von Mises part of the creep strain, and $\sigma_{y0}$ is the initial yield stress. A complete description of the underlying numerical method and associated verification exercises may be found in Ref. 62.

The objective of the computations is to employ Bayesian calibration to evaluate the creep constant $A_c$, assuming $B=20$, $m=1.0$ and $n=0=0.5$, values that are appropriate for Coble creep. The plate element model in MEMOSA-FVM is used for the computation. Fluid damping and dielectric charging are not included in the computation, the former because of the slowness of the creep response, and the latter because of the absence of a dielectric in the experiment. A plate element mesh of 3226 quadrilateral elements is used in the computation, based on a mesh convergence study; a typical mesh is shown in Fig. 5.17. A time step of one hour is used, again based on a time-step convergence study. The focus is on Stage II creep in Fig. 5.18. The membrane is initially held in its undeformed position, and a voltage of 20V is applied. The membrane is elastically deformed to the $t=0$ asymptote of the experimental data, as shown in Fig. 5.17. The creep deformation calculation then commences, with the plate mesh being deformed at each time step. A third-order generalized polynomial chaos fit in Hermite polynomials is used to construct a response surface of membrane center point deformation at time instants of 200, 400 and 600 hours. Typical response surfaces at the three time instants and the associated standard deviation (based on the error of the gPC surface reconstruction at the collocation points) are shown in Fig. 5.18. $A_c$ and Young’s modulus $E$ are the parameters of these surrogate models.
A Bayes network for the creep computation is shown in Fig. 5.19. The PDF of $E$ is obtained from mesoscale simulations, and hence only $A_c$ is calibrated. First, we consider the natural variability of $E$ and measurement uncertainty, and a uniform distribution is used as the prior PDF of $A_c$. Based on the calibrated PDF of $A_c$, predictions of deflection at the three time points can be made using the polynomial chaos surrogate models. As shown in Table 5.5, significant discrepancy exists between predictions and data, which indicates the existence of model error. To account for the discrepancy, a model form error term $\varepsilon_{mf}$ is introduced into the Bayes network, as shown in Fig. 5.19. By assuming uniform prior PDFs for both $A_c$ and $\varepsilon_{mf}$, posterior PDFs are calculated and are shown in Fig. 5.19. The calibrated PDF of $\varepsilon_{mf}$ suggests that the mean value of $\varepsilon_{mf}$ is around -0.5e-07 m, i.e., the model tends to overestimate the deflection. As shown in Table 5.5, the discrepancy between model predictions and data is reduced after introducing $\varepsilon_{mf}$.
5.6 Uncertainty Quantification of Coarse-Grained System Simulations

5.6.1 UQ of PRISM Device Lifetime Simulations

Time-to-failure predictions of the PRISM device were conducted during Year 3 using the coarse-grained model. The focus was on PRISM Generation 5 devices. The input parameters are given in Table 5.6. The devices have significant residual stresses, which are modeled in the simulation through an effective Young’s modulus. Two types of simulations were performed. First a single contact event was simulated to determine the sensitivity of pull-in time and pull-in velocity to input parameters. In the second type of simulation, multi-cycle static contact events were simulated to determine the influence of input parameters on dielectric charging, specifically on the pull-in and pull-out voltages, and the overall time to failure due to electrostatic stiction. The greatest sensitivity of the pull-in ($V_{PI}$) and pull-out voltages ($V_{PO}$) are to membrane length ($L_m$), gap, ($y_0$), thickness ($H_m$) and effective Young’s modulus ($E$). Time-to-failure ($T_{FAIL}$), which is determined by dielectric charging in these simulations, is again largely determined by these same parameters, though the dielectric thickness also contributes significantly. However, epistemic uncertainties in the dielectric charging model also play a big role, particularly the barrier height $\phi_B$, effective mass $m^*$ and the number of traps, $N_T$. The dynamics of the membrane are in large part determined again by the membrane geometry, and by the dielectric constant of the dielectric, $\varepsilon_r$.

A summary of results is given in Figs. 5.20, 5.21 and 5.22. Fig. 5.20 shows the sensitivity of outputs ($y$) to inputs ($u$), defined as:

$$\frac{|y_{\text{max}} - y_{\text{min}}|}{y_{\text{avg}}} \times \frac{u_{\text{avg}}}{|u_{\text{max}} - u_{\text{min}}|}$$

Fig. 5.19: Bayes network for creep calibration, and posterior distributions of creep constant and model form uncertainty.

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<table>
<thead>
<tr>
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</thead>
<tbody>
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</tr>
<tr>
<td>S. Palit, ECE, Purdue</td>
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</table>
The greatest sensitivity of the pull-in ($V_{PI}$) and pull-out voltages ($V_{PO}$) are to membrane length ($L_m$), gap, ($y_0$), thickness ($H_m$) and effective Young's modulus ($E$). Time-to-failure ($T_{FAIL}$), which is determined by dielectric charging in these simulations, is again largely determined by these same parameters, though the dielectric thickness also contributes significantly. However, epistemic uncertainties in the dielectric charging model also play a big role, particularly the barrier height $\phi_B$, effective mass $m^*$ and the number of traps, $N_T$. The dynamics of the membrane are in large part determined again by the membrane geometry, and by the dielectric constant of the dielectric, $\varepsilon_r$. Figs. 5.21 and 5.22 show PDFs of output parameters resulting from aleatoric uncertainties in key input parameters. A key result is that the PDF of the time-to-failure has a large spread, and predicting the mean to within one order of magnitude is not a trivial undertaking.

The coarse-grained model has provided important insights into the factors that control uncertainty in our predictions. Uncertainty in device dimensions is central to prediction uncertainty; this has emerged as the dominant theme across the range of simulations performed thus far. However, it is clear from both our coarse-grained simulations as well as more detailed dielectric charging UQ simulations in MEMOSA that model-form uncertainty in the dielectric charging model is also critical. Fabrication uncertainties are difficult to control, but can be characterized carefully, and the metrology efforts in PRISM Gen 5 have been designed to do this. The dielectric charging model has been enhanced to reflect the existence of multiple trap levels, and MEMOSA simulations using this new model will be undertaken in Year 4.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mean</th>
<th>St. Deviation</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_m$: Membrane Length ($\mu$m)</td>
<td>500</td>
<td>10</td>
<td>Measurements</td>
</tr>
<tr>
<td>$H_m$: Membrane Thickness ($\mu$m)</td>
<td>1.85</td>
<td>0.3</td>
<td>Measurements</td>
</tr>
<tr>
<td>$E$: Young modulus (GPa)</td>
<td>350</td>
<td>80</td>
<td>Measurements</td>
</tr>
<tr>
<td>$y_0$: Airgap ($\mu$m)</td>
<td>3.5</td>
<td>0.26</td>
<td>Measurements</td>
</tr>
<tr>
<td>$y_d$: Dielectric Thickness (nm)</td>
<td>191</td>
<td>16</td>
<td>Measurements</td>
</tr>
<tr>
<td>$\varepsilon_r$: Dielectric constant (-)</td>
<td>7.9</td>
<td>0.5</td>
<td>Literature/Guess</td>
</tr>
<tr>
<td>$\phi_B$: Barrier Height (eV)</td>
<td>1.5</td>
<td>0.2</td>
<td>Measurements</td>
</tr>
<tr>
<td>$N_T$: Trap density (cm$^{-3}$)</td>
<td>2e18</td>
<td>1e18</td>
<td>Measurements</td>
</tr>
<tr>
<td>$\sigma$: Capture cross section (cm$^2$)</td>
<td>1e-17</td>
<td>5e-18</td>
<td>Literature/Guess</td>
</tr>
<tr>
<td>$m^*$: Effective mass (-)</td>
<td>0.5</td>
<td>0.2</td>
<td>Measurements</td>
</tr>
<tr>
<td>$\gamma$: FP attempt frequency (s$^{-1}$)</td>
<td>1e12</td>
<td>5e11</td>
<td>Literature</td>
</tr>
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</table>

Table 5.6: Input parameters for uncertainty quantification in coarse-grained model simulations of membrane dynamics and dielectric charging
Fig. 5.20: Sensitivity of outputs to inputs using coarse-grained model. (a) Pull-in and pull-out voltage, (b) time to failure, and (c) time to pull-in and pull-in velocity. Uncertainties in device geometry, as well as model form uncertainty in the dielectric charging model have emerged as the primary determinants of prediction uncertainty.

Operating Voltage=80V

Fig. 5.21: PDFs of pull-in time and pull-in velocity resulting from aleatoric uncertainties in inputs.
5.6.2 Multiscale Simulation of Pull-in and Pull-out with Quantified Uncertainty

The prediction of pull-in and pull-out voltages of the PRISM device are central to the three Year 5 predictive goals of the center. During the reporting period we integrated a multiscale model for pull-in and pull-out involving device-level simulations, a mesoscale contact model and atomistic simulations (molecular dynamics and ab initio density functional theory), as shown in Figure 5.23. The goal of the effort was to develop and exercise PRISM’s uncertainty quantification framework before performing fully-resolved simulations.

The multiscale model is based on first principles calculations and calibration experiments, including device geometry and surface roughness. At the finest-grained level, atomistic computations are used to provide elastic properties and size-dependent plasticity of contacts. These provide inputs to the mesoscale contact model described in previous sections. This model, in turn, forms the contact model used in coarse-grained simulations of pull-in. The device-level coarse-grained model uses Euler-Bernoulli beam theory, together with a fluid damping correlation integrating the ES-BGK model for

Table 5.7: Sensitivity of the pullout voltage to inputs. The last column shows the gradient of the quantity of interest multiplies by the range.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Range</th>
<th>Source</th>
<th>dQoI/dx</th>
<th>Sens * Uncert</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometric parameters</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Beam length (microns)</td>
<td>[694.4 - 495.8]</td>
<td>PRISM - Mic</td>
<td>~0</td>
<td>~0</td>
</tr>
<tr>
<td>Beam thickness (microns)</td>
<td>[1.60 - 1.85]</td>
<td>PRISM - Mic</td>
<td>2.32E+06</td>
<td>0.58</td>
</tr>
<tr>
<td>Die. Length (microns)</td>
<td>[2.12 - 2.12]</td>
<td>PRISM - Mic</td>
<td>3.0E+04</td>
<td>0.07</td>
</tr>
<tr>
<td>Die. Thickness (nm)</td>
<td>200</td>
<td>PRISM - Design</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Residual stress (MPa)</td>
<td>[8.5 - 17.5]</td>
<td>PRISM - BayesCal</td>
<td>3.10E-01</td>
<td>2.79</td>
</tr>
<tr>
<td>Materials properties</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Beam’s Young’s mod (GPa)</td>
<td>[180 - 220]</td>
<td>PRISM - XRD/Theo</td>
<td>8.46E-12</td>
<td>0.34</td>
</tr>
<tr>
<td>Creep rate (e-7 1/s)</td>
<td>5.44/-1.3</td>
<td>PRISM - BayesCal</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Contact</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Contact height (nm)</td>
<td>[100 - 140]</td>
<td>PRISM - MesoContact</td>
<td>4.74E+07</td>
<td>1.89</td>
</tr>
</tbody>
</table>

Fig. 5.22: PDFs of pull-in voltage, pull-out voltage and number of cycles to failure as a function of input aleatoric uncertainties.
rarefied gas dynamics. This model was extended to determine the role of different degradation mechanisms (such as creep) and the lifetime of PRISM switches (characterized by the variation of pull-in and pull-out voltages with operation time and conditions). Extensions include: i) a creep-enhanced Euler-Bernoulli beam model to describe the time-dependent response of the device membrane; ii) residual stress, and iii) a physics-based contact model to describe the interaction between the two surfaces. This multiscale model forms the central core for which uncertainty quantification is performed.

Table 5.7 shows a linear sensitivity analysis of the device level model showing all variables, their uncertainty and origin, for a single contact even simulation. The model includes the elastic response of the membrane, creep (which does not play an important role for the short time-scale simulations in this table) and fluid damping. Dielectric charging is not included in the table, again because of the short simulation time scale. The sensitivity analysis show that the average separation between the two contacting surfaces (associated with surface roughness and properties) and residual stress (obtained via Bayesian calibration) play dominant roles in the prediction of the quantity of interest, in this case, the pull-in voltage.

**Pull-in and Pull-out Voltage.** Our simulations involve switch closing by the application of an external electrostatic force, which is proportional to the square of the applied voltage and inversely proportional to the square gap between top membrane and dielectric landing path. Pull-in and pull-out voltages are defined as the voltages needed for the gap to reach 10 nm during closing and opening, respectively. We determined the pull-in voltage of the nominal Generation 5 device to be 70 V in absence of creep (device

---

Fig. 5.23: Multiscale model for pull-in voltage.
dimensions are shown on the left portion of Fig. 5.24. Figure 5.25 shows how uncertainties in geometry, and the multiscale contact model are captured and propagated to predict the pull-out voltage with all uncertainties quantified.
Role of Creep: In addition to the single-contact even simulations described above, we also performed creep simulations using the coarse-grained model spanning hundreds of hours. For sub-pull-in voltages applied over a long period of time, creep leads to a reduction in gap with the associated increase in electrostatic force; this process leads, in time, to pull-in. Our preliminary results show that creep time required to pull-in increases super-exponentially with applied voltage. Figure 5.26 shows how creep deformation affects the pull-in (left panel) and pull-out (right) as a function of the time for which a pre-pull voltage is applied. The simulation results for different applied voltages, and the apparent saturation observed for 55 V, are consistent with the super-exponential dependence of creep time observed in Fig. 5.24.

These computations using the coarse-grained model have demonstrated how the integration of atomistic, mesoscale and device-level models can be carried and how uncertainties can be propagated across scales in a PRISM device simulation. Ongoing experiments will provide validation data that will be used with Bayesian analysis to assess the accuracy of our predictions and identify avenues to improve our predictive capabilities if necessary.
6. EXPERIMENTAL PROGRAM
We now describe the main achievements of our experimental program to provide characterization and validation data.

6.1 Frogleg Creep Experiments
During Year 3, capacitive creep measurements on electroplated nanocrystalline nickel plates were conducted for 100s-1000s hours using (i) the AD7746 capacitance to digital converter (<200 aF uncertainty of the test setup offers a 10 nm height uncertainty) and (ii) a direct optical measurement using a confocal microscope from Olympus (LEXT OLS3100). A square wave bias was applied with a >98% duty cycle of to collect both the on-state and off-state deflection measurements. Fig. 6.1 shows an example of the recorded measurements for a frog-leg structure. The creep mechanisms in nanocrystalline nickel were explained to be diffusion at 20°C (Coble creep) based on the model developed by Prof. Koslowski. More optical measurements using the Olympus LEXT confocal microscope are underway on the PRISM device to further validate the models, and for UQ.

![Fig. 6.1: Measured gap and capacitance in creep measurements for frog-leg device.](image)

6.2 Extraction of Geometric Parameters
Sensitivity analysis using our coarse-grained solver indicates that aleatoric uncertainty related to device geometry is a central determinant of prediction uncertainty. Significant effort has been dedicated in Year 3 to obtaining statistical characterization of important geometric parameters of the PRISM device. The most important geometric parameters of the Gen 5 PRISM device are shown in Fig. 6.2. These geometric parameters are measured optically using a confocal laser scanning microscope, LEXT OLS3100, from Olympus. The measurement uncertainties and measured geometric data are summarized in Table 6.1. The values for all geometric parameters exhibit normal distributions and thus mean values and standard deviations are used to represent the fabrication variation across the wafer.

![Researchers](image)

Researchers
- H. H. Hsu, ECE, Purdue
- M. Koslowski, ME, Purdue
- A. Kovacs, ECE, Purdue
- A. Kumar, Ece, Purdue
- D. Peroulis, ECE, Purdue
- J. Small, ECE, Purdue
6.3 Residual Stress Extraction based on Model

Residual stress characterization is a critical part of PRISM switch modeling since it determines the degree of deflection that a given electrostatic force engenders. Direct measurements of residual stress are difficult to make and efforts are underway to devise experiments to isolate residual stress effects (see Section 6.4 below). In order to obtain an idea of the level of residual stress and its relation to the fabrication process, we extracted residual stress through careful modeling of membrane deformation during pull-in. In the present effort, the residual stress is extracted by iterating its value in a comprehensive 1-D beam model. A line-search algorithm in the Matlab optimization toolbox is used, and the residual stress value iterated until the best fit between the measured and modeled displacement versus voltage curves is found. Figure 6.3 shows a flowchart of the optimization process.

The underlying coarse-grained model accounts for residual stress, membrane curvature,
fringing field effects and non-ideal anchors. Figure 6.4 shows an example of measured beam profile and the approximate beam model used in the 1-D simulation. The middle section of the profile curves up where there is actuation electrode beneath it. The edge of the anchor is not ideally straight, but rises gradually with a slope of about $10^\circ$. This angle is modeled as a torsional spring. The non-flat profile of the beam is approximated by a finite Fourier sine series with twelve terms.

In order to quantify the residual stress distribution on the wafer, the displacement-versus voltage curves for 90 membranes on a 4-inch quarter-wafer are measured. We assume a value of Young’s modulus $E = 199.9$ GPa, which is smaller than the bulk material value $E = 221$ GPa since value for the electroplated nickel film is related to the plating condition. For all the 90 membranes measured, the location of the membranes on the wafer and the scalar-scaled results of the extracted residual stress are shown in Figure 6.5(a), and all values of the extracted residual stress are plotted in a histogram in Fig. 6.5(b). Here, positive values represent tensile stress while negative ones denote compressive stress. The values of residual stress exhibit a normal distribution with a mean of 5.69 MPa and standard deviation of 5.05 MPa. The results show that most membranes have tensile stress.

![Fig. 6.4: Measured beam profile and non-ideal beam model.](image)

![Fig. 6.5: (a) Distribution of residual stress across wafer, and (b) histogram of measured residual stress.](image)
6.7 AFM-Based Measurements of Residual Stress

Characterization of the residual stress in the PRISM is difficult because membrane displacement is a function of both membrane material and geometric properties as well as the residual stress resulting from the fabrication process. During Year 3, experiments were devised which could separate these two effects. Simulations by Prof. Sulsky’s group show that for small deformation, the stiffness at the center \((k_s)_{\text{center}}\) and the unfixed edge \((k_s)_{\text{edge}}\) of the PRISM membrane are both approximately linear functions of membrane thickness \(t\) and the residual stress \(\sigma\). Thus \(t\) and \(\sigma\) can be extracted from the measurement of \((k_s)_{\text{center}}\) and \((k_s)_{\text{edge}}\).

The experimental work consisted of measuring the stiffness of the PRISM fixed-fixed devices at the center and the unfixed edge using AFM force versus distance curves. Ten devices (five 500μm long devices and five 400μm long devices) were tested using an Agilent 5500 AFM; two sets of force versus distance curves were taken at the center and the unfixed edge respectively for each device (see Fig 6.6 (a)). The slopes of the converted force versus deformation curves give the local stiffness of the devices (see Fig 6.6(b)). These data will be used to calibrate the thickness and residual stress of the device in Year 4, and will provide an independent measure of residual stress to compare to the model-based extraction described above, and PDFs obtained by Bayesian calibration.

6.8 Measurement of Transient Membrane Response

During Year 3, experiments commenced on the measurement of the transient response of the PRISM Gen 5 membrane during pull-down, contact and pull-out. In these experiments, a voltage pulse with maximum voltage greater than the dynamic pull-in voltage is applied, and the deformation of the membrane mid-point is measured as a function of time. Figure 6.7(a) shows the experimental set-up in which the RF-MEMS switch is placed inside a vacuum probe station and its transient response is measured by a laser Doppler vibrometer. Measurements were made using a Suss vacuum
probe station and Polytec MSA-400 scanning laser Doppler vibrometer. Figure 6.7(b) shows the measured membrane, with the location of the laser spot in red.

Figures 6.8 (a) and (b) show the velocity of the membrane mid-point as a function of time (blue) for a 100 V step voltage pulse (green); the experiment was conducted at an ambient pressure of 5 Torr. The corresponding displacement versus time curve is shown in Fig. 6.8(b). These experiments will be repeated over multiple devices and multiple replicates in Year 4 for a range of voltage inputs and ambient pressures. The data will then be processed to obtain the maximum velocity reached by the switch before impact, and the time to the first velocity reversal. This data will be used to validate the PRISM full system contact simulations.
The primary goal of the Year 3 work was to predict the in-plane Young’s modulus of the electroplated nickel membrane in the PRISM switch by measuring its crystallographic texture using X-ray diffraction (XRD) and calculating three different polycrystal elasticity averages, the Voigt, Reuss, and Hill averages. These three averages are based on the principle that the elastic response of a polycrystalline sample (e.g., the nickel membrane) can be estimated by averaging the single crystal elastic tensor of the material (e.g., nickel) over the orientation distribution of crystallites in the sample. Details of the Voigt, Reuss, and Hill polycrystal elastic averages may be found in the original papers or in the classic text on texture analysis by Kocks et al.

XRD measurements of electroplated nickel films of different thicknesses showed that the 001 type fiber texture increased as a function of thickness, which suggests that the in-plane Young’s modulus is a function of height within the film. However, XRD could not be used to quantify the increase of texture strength as a function of film height within the nickel film, which is only ~3 µm thick, due to the poor depth resolution of XRD texture measurements. Therefore a specialized transmission electron microscopy (TEM) technique was developed to measure the increase in 001 texture as a function of
height within a single nickel film from an RF MEMS switch. Details of the TEM technique can be found in Ref. 67.

6.9.1 In-plane Young’s Modulus

It is well-known that elastic properties such as Young’s modulus are not affected by micro-scale size effects in MEMS devices. However, crystallographic texture does influence elastic properties and the Young’s modulus of polycrystalline films in MEMS can be predicted if the crystallographic texture is known.

Texture measurements on individual RF MEMS switches were made using two-dimensional (2D) X-ray diffraction on a laboratory Bruker GADDS diffractometer equipped with a Hi-Star multiwire proportional counter (MWPC) area detector, a 2-position chi stage, Cu Ka radiation, and a 0.5 mm monopillar for microdiffraction. The monopillar incident optics produce an incident X-ray beam with a diameter small enough to irradiate a single RF MEMS switch, thereby allowing texture quantification of the nickel bridge in individual MEMS.

The Rietveld refinement software MAUD was used to perform texture analysis and generate recalculated pole figures which were exported for further analysis and plotting in MTEX, a MATLAB toolbox for texture analysis. MTEX was used to calculate the Voigt, Reuss, and Hill average in-plane Young’s modulus for the nickel membrane in 20 different RF MEMS switches (10 switches from each batch). An inverse pole figure from a representative nickel membrane is shown in Fig. 6.9.

![Fig. 6.9: Inverse pole figure (normal direction) from the nickel bridge of an RF MEMS switch. Contour lines every 0.5 m.r.d. (multiple of a random distribution).](image)

<table>
<thead>
<tr>
<th>Perfect 001 Texture</th>
<th>RF MEMS Switches (batch #1)</th>
<th>RF MEMS Switches (batch #2)</th>
<th>Uniform Texture</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{\text{in-plane}}^{\text{Reuss}}$</td>
<td>163.3</td>
<td>178.8 $\pm$ 1.1</td>
<td>183.3 $\pm$ 1.0</td>
</tr>
<tr>
<td>$E_{\text{in-plane}}^{\text{Hill}}$</td>
<td>172.4</td>
<td>194.7 $\pm$ 1.3</td>
<td>199.9 $\pm$ 1.1</td>
</tr>
<tr>
<td>$E_{\text{in-plane}}^{\text{Voigt}}$</td>
<td>182.7</td>
<td>210.3 $\pm$ 1.5</td>
<td>216.1 $\pm$ 1.2</td>
</tr>
</tbody>
</table>

Table 6.2: Reuss, Voigt, and Hill average in-plane Young's modulus ($E_{\text{in-plane}}$) predicted by XRD measurements.

The Voigt average effectively assumes constant strain in the crystallites in a polycrystal and therefore represents an upper bound, while the Reuss average assumes constant stress. The Hill average, which is a geometric average of the Voigt and Reuss averages, has been shown to provide estimates of elastic properties reasonably close to experimental values for polycrystals of materials with low to moderate elastic anisotropy. All three averages are presented in Table 6.2. The Hill average is expected to be most representative of the actual in-plane Young’s modulus of the nickel bridges. The Reuss and Voigt values are lower and upper bounds, respectively. For comparison, the in-plane Young’s modulus for a hypothetical nickel bridge with perfect 001 fiber texture is presented along with the in-plane Young’s modulus for a nickel film with a uniform texture (i.e., no texture).
Switches from batch #1 are predicted to have an average in-plane Young’s modulus of 194.7 GPa +/- 1.3, while switches from batch #2 have an average in-plane Young’s modulus of 199.9 GPa +/- 1.1. The slight difference from batch to batch is due to a stronger 001 type fiber texture in batch #1.

6.9.2 In-plane Young’s Modulus as Function of Film Height
A specialized hollow-cone dark field TEM technique was developed to measure crystallographic texture as a function of film height within the nickel bridge film from a single RF MEMS switch. The technique cannot measure the full range of crystallite orientations, but rather a select few orientations of interest, including crystallites whose 001 crystallographic planes are perpendicular to the film normal direction, i.e., those crystallites that have 001 fiber texture.

It was discovered that degree of 001 crystallographic texture increased approximately linearly as function of height within the nickel membrane, as shown in Fig. 6.10. It is impossible to calculate direct Reuss, Voigt, and Hill averages based on this data because the TEM technique does not measure the full crystallite orientation distribution. If some assumptions are made about the nature of the orientation distribution, it can be estimated that the effect of the texture evolution with film height is to produce an in-plane Young’s modulus that varies with film height, from 210 GPa at the bottom of the film (the bulk isotropic value for nickel) to 180 GPa at the top of the film. It is expected that the in-plane Young’s modulus varies roughly linearly as a function of film height.

6.10 Thermal Characterization of PRISM Membrane
During Years 2 and 3, our research focused on characterizing the performance of the PRISM device under powered operation. The small length scales of microelectromechanical systems (MEMS) often lead to high current densities that can result in local temperature rises of hundreds of degrees Kelvin. In order to predict the thermal, mechanical and electrical performance of these microdevices under powered operation, accurate material property information is essential. Although bulk thermal properties of materials are readily available in the literature, materials tend to exhibit different thermal properties when length scales are reduced to microscale dimensions because of boundary and/or microstructural effects. Here, we present electrical and thermal measurements conducted on PRISM RF MEMS switches in order to extract material properties and predict the effect of self-heating on the switch’s actuation voltage. Increased electrical resistivity and decreased thermal conductivity in comparison to bulk values are reported for the devices. DC electrical self-heating is monitored using infrared (IR) thermography. The finite volume method is used to determine thermal conductivity by a fit to the measured temperature profiles. Additionally, microbridge deflection during self-heating is measured with a laser confocal microscope. Computer simulation of the deflected profiles is used to determine the change in actuation voltage of the switches.

An IR microscope system capable of measuring two dimensional surface temperature profiles with a spatial resolution of 2 μm at the AFRL/RXBT laboratory facility was employed to conduct thermal

<table>
<thead>
<tr>
<th>Researchers</th>
</tr>
</thead>
<tbody>
<tr>
<td>A. Bajaj, ME, Purdue</td>
</tr>
<tr>
<td>T.S. Fisher, ME, Purdue</td>
</tr>
<tr>
<td>D. Peroulis, ECE, Purdue</td>
</tr>
<tr>
<td>R. Sayer, ME, Purdue</td>
</tr>
</tbody>
</table>
mapping. Temperature profiles of eight, generation 4 PRISM devices (microbridges) subjected to DC heating were obtained. Fig. 6.11(a-d) shows the thermal maps obtained for one of the devices under DC biases ranging from 300 to 600 mA. The centerline temperature profiles averaged over the eight tested samples as well as the corresponding standard deviations are shown in Fig. 6.11(e). Under ideal conditions the maximum temperature rise should occur at the center of the beam and the smallest temperature rise should be at the ends of the beam, which is consistent with the trends observed in Fig. 6.11.

The temperature profiles on the Ni microbridge shown in Fig. 6.11(e) were fit to the thermal model shown below using the finite volume method:

\[
k A_\text{c} \frac{d^2 T}{dx^2} + \frac{I^2 R}{L} - \varepsilon \sigma (T^4 - T_\text{a}^4) - hP (T - T_\text{a}) = 0
\]

where \(k\), \(A_\text{c}\), and \(P\) are the thermal conductivity, cross-sectional area, and perimeter of the Ni microbridge. \(I\) is current, \(R\) is resistance, \(\varepsilon\) is emissivity, \(h\) is the heat transfer coefficient, \(T\) is temperature and \(T_\text{a}\) is ambient temperature. In the above equation, thermal conductivity is the only unknown. From a best fit, the thermal conductivity of the Ni is found to be 72.6 ± 1.2 W/mK, where the uncertainty is found using bootstrapping. The measured thermal conductivity is 20% below that of bulk Ni (91 W/mK) and in good agreement with the theoretical value of 79.9 W/mK for a film with a grain size of 50 nm.

The electrical resistivity of the electroplated Ni microbridges was found to be 9.7 ± 0.3 \(\mu\Omega\)cm. This value is 38% greater than bulk Ni. A simple Wiedemann-Franz analysis using the measured electrical resistivity reveals an electronic thermal conductivity of 74.6 W/mK at room temperature, in close agreement with our thermal measurement. The slightly lower measured thermal conductivity may be the result of higher average microbridge temperatures during the thermal experiments. The fact that the measured resistance is 38% more than the cited bulk value while the thermal conductivity is only 20% less than the cited bulk thermal value is likely due to differences in between the bulk samples for the respective tests. Further, we note that phonon thermal conductivity, which accounts for approximately 8% of overall thermal conductivity in bulk Ni, is not captured by the Wiedemann-Franz analysis.
Self-heating during operation will cause thermal expansion of the Ni film. The anchor points of the microbridge resist the expansion of the film, thus giving rise to thermal compressive stress that causes the beam to deform in the vertical direction. As the microbridge deforms, the gap between the suspended film and the actuation electrodes increases. The average centerline profile of the microbridges is shown in Figure 6.12(a) for heating currents ranging from 0 to 550 mA. Initially, the beam is not perfectly flat, but rather it is curved upwards in the center due to the profile of the actuation electrodes during fabrication. As the heating current is increased, the beams deflect upwards, increasing the overall gap between the microbridge and substrate. Under maximum heating, the center of the beam (x = 0) deforms 1.6 µm upwards. The increased gap height can have a profound effect on the pull-in voltage required to actuate the switch in the ON state.

A one-dimensional beam model that incorporates residual stress, non-linear stretching, plate-like bending, squeeze film damping, electrostatic force and beam/substrate impact developed by Snow and Bajaj was used to simulate the pull-in voltage required to actuate the switch to the ON state. Figure 6.12(b) shows the simulated pull-in voltages for the beam profiles of Fig. 6.12(a). For the zero heating case (I = 0 mA), 130 V is required to actuate the switch. A significant increase in actuation voltage is computed as the heating current in the microbridge is increased. At the maximum applied current of 550 mA, the pull-in voltage is 230 V, a 79% increase from the unheated microbridge. These results show that self-heating must be accounted for in the design process to ensure proper operation of electrostatically actuated MEMS switches.

Fig. 6.12: (a) Gap height along the centerline of the Ni microbridge for different self-heating currents. (b) Simulated pull-in voltage of the switch as a function of self-heating current.
7. UNCERTAINTY QUANTIFICATION METHODS

7.1 Data Driven Framework for UQ

During Year 3, we developed a data-driven stochastic collocation approach to include the effect of uncertain design parameters during complex multi-physics simulation of micro-electro-mechanical systems (MEMS). The proposed framework is comprised of two key steps: first, probabilistic characterization of the input uncertain parameters based on available experimental information, and second, propagation of these uncertainties through the predictive model to relevant quantities of interest. The uncertain input parameters are modeled as independent random variables, for which the distributions are estimated based on available experimental observations, using a nonparametric diffusion-mixing based estimator. The diffusion-based estimator derives from the analogy between the kernel density estimation (KDE) procedure and the heat dissipation equation and constructs density estimates that are smooth and asymptotically consistent. The diffusion model allows for the incorporation of the prior density and leads to an improved density estimate, in comparison with the standard KDE approach. We have demonstrated this through several numerical examples. Following the characterization step, the uncertainties are propagated to the output variables using the stochastic collocation approach, based on sparse grid interpolation. We have used the data-driven framework to

Fig. 7.1: (Top row) Density estimates and experimental observations ($M=33$) for Young’s modulus of polysilicon films resulting from heterogeneous measurements. (a) Young’s modulus values as measured by various researchers using different measuring techniques and (b) density estimates using standard KDE and diffusion model. (Bottom row) Effect of variability in input parameters on MEMS switch: probability density function (PDF) of vertical tip deflection for various applied voltages. (a) Applied voltage $V=3.0V$ and (b) applied voltage $V=6.0V$. 

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study the effect of variations in Young’s modulus, induced as a result of variations in manufacturing process parameters or heterogeneous measurements on the performance of a MEMS switch (see Fig. 7.1).

7.2 Improved Sparse Grid Techniques
We also developed efficient techniques for numerical solution of differential equations with random inputs, defined on bounded random domain with non-uniform probability measures. Recently, there has been a growing interest in the stochastic collocation approach, which seeks to approximate the unknown stochastic solution using polynomial interpolation in the multi-dimensional random domain. Existing approaches employ sparse grid interpolation based on the Smolyak algorithm, which leads to orders of magnitude reduction in the number of support nodes as compared with usual tensor product. However, such sparse grid interpolation approaches based on piecewise linear interpolation employ uniformly sampled nodes from the random domain and do not take into account the probability measures during the construction of the sparse grids. Such a construction based on uniform sparse grids may not be ideal, especially for highly skewed or localized probability measures. To address this issue, we developed a weighted Smolyak algorithm based on piecewise linear basis functions, which incorporates information regarding non-uniform probability measures, during the construction of sparse grids. The basic idea is to construct piecewise linear univariate interpolation formulas, where the support nodes are specially chosen based on the marginal probability distribution. These weighted univariate interpolation formulas are then used to construct weighted sparse grid interpolants, using the standard Smolyak algorithm. This algorithm results in sparse grids with higher number of support nodes in regions of the random domain with higher probability density (Fig. 7.2).

Fig. 7.2: Normalized error in mean versus number of grid points N for Genz test functions \([n=2, y_i \sim \text{Beta}(10, 1), i = 1, 2]\), using uniform and weighted Smolyak algorithms.
Novel Hybrid Algorithm for Failure Probability Estimate

Computing failure probability is a critical task in many problems such as reliability analysis, risk management, etc. The goal is to compute the following failure integral.

\[ P_f = \int_{g(Z)<0} \rho(Z) dz, \]

where \( g(Z) \) defines failure. The failure mode \( g<0 \) usually is not known analytically and can only be computed numerically, which requires a full system simulation. During this year, we developed a novel hybrid algorithm. It is based on using a surrogate model of \( g \) to sample in the large portion of the random space reasonably “away” from the failure mode and using the samples of the true system “close” to the failure mode. As a result, the hybrid algorithm is robust, in the sense that it will always produce accurate result, and is efficient, in the sense that it uses far fewer samples than Monte Carlo simulation (MCS) does. A rigorous mathematical analysis was conducted and the convergence of the hybrid algorithm was established in a theorem in Ref. 85. From an implementation point of view, we demonstrate that accurate surrogate models such as those based on generalized polynomial chaos (gPC) show great advantage. However, the hybrid algorithm works well for any surrogate models with finite accuracy. For example, consider a limit state function

\[ g(Z) = Z_1 + 2Z_2 + 2Z_3 + Z_4 - 5Z_5 - 5Z_6 + 0.001 \sum_{i=1}^{6} \sin(100Z_i), \]

where each \( Z_i \) is a lognormal random variable. We use Hermite gPC to approximate the function and drop the sine function. Thus the constructed gPC surrogate has a finite error that will not vanish. (This is done intentionally to emphasize the fact that the hybrid algorithm works for any surrogate.) The results are summarized in Table 7.1. The “exact” solution is obtained by MCS with \( 10^6 \) samples. We observe that with the hybrid algorithm, we obtain highly accurate results with just a few hundred samples. With a sufficiently accurate gPC model, i.e., \( N=9 \), with only 600 samples, we reproduce exactly the MCS solution with \( 10^6 \) samples. Thus, for the first time, we have a highly accurate algorithm for failure probability estimation that is suitable for practical complex systems.

<table>
<thead>
<tr>
<th>gPC order</th>
<th>3</th>
<th>5</th>
<th>7</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. of samples</td>
<td>18,600</td>
<td>200</td>
<td>400</td>
<td>600</td>
</tr>
<tr>
<td>Error</td>
<td>$4.2 \times 10^{-3}$</td>
<td>$4.9 \times 10^{-4}$</td>
<td>$1.1 \times 10^{-4}$</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 7.1: Errors of gPC hybrid algorithm for failure probability estimation.

Hybrid Algorithm for Rare Failure Probability

A much more useful task is to estimate rare failure probability, that is, failure probability no bigger than \( 10^{-5} \). In this case, there exist no general non-sampling methods that are effective. This is because all existing non-sampling methods such as FORM and SORM are not accurate enough to resolve such a small probability. The only reliable approach is Monte Carlo Sampling (MCS), which requires \( 10^9 \) samples. Clearly this is out of the reach of any practical systems. To alleviate this difficulty, importance sampling (IS) is often used. With the best IS technique, one can usually reduce the number of samples to \( 10^5 \), which is still beyond our simulation capability for complex systems. In summary, for rare failure probability, there exist no effective simulation algorithms. In this project, we extended the hybrid algorithm by combining it with an effective IS technique. In particular, we employ the cross-entropy (CE) IS method. Our preliminary study demonstrated that the CE based hybrid algorithm can effectively simulate rare failure probability with only a few hundred simulations.
Consider the example from Section 7.3. We adjusted the parameter values such that the true failure probability is around $2 \times 10^{-6}$. The results by the CE based hybrid algorithm are shown in Table 7.2. We observe that again with just a few hundred simulations, the algorithm is able to produce highly accurate estimates of such a small probability. Thus, the method makes it possible for the first time to accurately estimate rare failure probability for complex systems.

<table>
<thead>
<tr>
<th>gPC order</th>
<th>2</th>
<th>4</th>
<th>6</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. of samples</td>
<td>1,600</td>
<td>400</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>Error</td>
<td>$2.12 \times 10^{-6}$</td>
<td>$2.07 \times 10^{-6}$</td>
<td>$2.09 \times 10^{-6}$</td>
<td>$2.08 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

Table 7.2: Estimating rare failure probability by cross-entropy based hybrid algorithm.
In this section, we describe the accomplishments of the thrusts described in Section 3.

### 8.1 Multiscale Dielectric Charging Model for RF-MEMS

Stiction failure due to dielectric charging in RF-MEMS is one of the most important reliability concerns. During Year 3, atomistic inputs were incorporated into our dielectric charging model to create a multiscale model. An overview of the approach we have taken is given in Fig. 8.1. Essentially, we start with electrons and atoms and the fundamental theories of quantum mechanics that govern their behavior, and predict bulk amorphous systems and the charge trapping characteristics of the defects contained within them. Once determined, these charge levels are used in a meso-scale dielectric charging model and ultimately predict dielectric breakdown.

We first describe the meso-scale model; details of the atomistic determination of trap depths are

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**Fig. 8.1**: Overview of dielectric charging modeling approach. Device-level simulations employ a mesoscale model of dielectric charging which requires the trap depth as a parameter. Molecular dynamics is used to predict defect structures, and point defects are identified and classified. Ab-initio charge state calculations are then performed to predict the trap depth distribution, which is then incorporated into a multi-trap depth meso-scale dielectric charging model.

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**Fig. 8.2**: Description of the charging model. Schematic of the dielectric band-diagram indicates the most important trapping/de-trapping current fluxes. First-order differential equations can be analytically solved to obtain expressions for leakage current and trap occupancies.

---

\[
\begin{align*}
J_{in} &= A_{in} (N - n_T) \\
J_{out} &= A_{out} n_T \\
J_e &= A_e n_T \\

\text{Injection:} \\
\text{Leakage:} \\
\text{Emission:}
\end{align*}
\]

\[
\begin{align*}
A_{in} &= \frac{N_T}{A_{in}} \\
A_{out} &= \frac{n_T}{A_{out}} \\
A_e &= \frac{n_T}{A_e}
\end{align*}
\]

**Trap Occupancy:**

\[
n_T(x, t) = \frac{A_{in}(x) N_T}{A_{out}(x)} \left(1 - \exp\left(-\frac{t}{q} A_{in}(x)\right)\right)
\]

**Steady state leakage:**

\[
J_s = \sum_x A_{in}(x) A_e(x) N_T \\
A_{out}(x) \\
A_{in}(x)
\]

\[
J_s = \sum_x \frac{A_{in}(x) A_e(x) N_T}{A_{out}(x)} \exp\left(-\frac{t}{q} A_{in}(x)\right)
\]

---

**Fig. 8.2**: Description of the charging model. Schematic of the dielectric band-diagram indicates the most important trapping/de-trapping current fluxes. First-order differential equations can be analytically solved to obtain expressions for leakage current and trap occupancies.
Models existing currently in literature are generally empirical, based on curve-fitting techniques applied to experimental data. Instead, we have developed a multiscale model based on physical dielectric electronic parameters to describe charge accumulation and current injection through a typical RF-MEMS dielectric for use in MEMOSA. The essential elements of the model are shown in Fig. 8.2. Furthermore, we have demonstrated the use of this model by integrating it with our coarse-grained solver. The latter employs the Euler-Bernoulli beam equation for a fixed-fixed membrane. Uncertainty quantification of PRISM device lifetime and output sensitivities were explored, as described in previous sections.

Since the dielectric charging is an exponential function of applied voltage, it is important to identify and characterize the most sensitive parameters used in the charging model (in this case barrier height, trap-depth and effective mass). A new method to extract barrier height and trap-depths from current transients was developed (Fig. 8.3), and the results verified against density functional theory (DFT) simulations (see below). Other electronic parameters for the dielectric are estimated from matching current transients measured at different voltages and temperatures. Based on known process variations and reasonable guesses for other input parameters to the charging model, a lifetime PDF can be obtained for the device (Fig. 5.22). To allow process and device

\[
\text{Reliability:} \\
\tau(x) = \frac{A_{w}(x) N_{T}}{A_{sw}(x) \left(1 - \exp \left( - \frac{t}{\tau} \right) \right)} \\
V_{p0}(t) = V_{p0}(0) - \frac{\int_{0}^{t} x n_{T}(t, x) dx}{e_{r} e_{0}}
\]

Fig. 8.4: Comparison of pull-out voltage shifts obtained numerically from the full simulation (FS) and from the coarse-grained model (CG).
engineers to quickly design a RF-MEMS device with specified performance and reliability metrics, we have developed a compact model to calculate actuation voltages, charge accumulation inside the dielectric and consequently failure time. The compact model (Fig. 8.4) has been verified against numerical simulations.

8.1.1 Atomistic Determination of Trap Depths
We now describe our approach to computing the trap depth $\Phi_t$ in the dielectric charging model shown in Figs. 8.1 and 8.2. We have developed a novel two-step multiscale approach which has already led to important predictions in both amorphous silicon dioxide ($a$-SiO$_2$) and amorphous silicon nitride ($a$-Si$_3$N$_4$). The two-step approach involves generating amorphous samples through a melting and quenching molecular dynamics (MD) procedure followed by further electronic relaxation via density functional theory (DFT). The validation of these amorphous samples to experimental structures can be achieved through comparisons of the densities and the radial distribution functions (RDFs). This has been done and is shown in Figs. 8.5 and 8.6. Once the structures are obtained, the defects are located and the formation energies calculated. From these calculations we have quantified the formation energy uncertainty by varying the choice of the DFT functional between the two most commonly used extremes, the local-density approximation (LDA) and the generalized-gradient approximation (GGA). A histogram showing this variation for two unique defects in silica is shown in Fig. 8.7.

Finally, using techniques analogous to those used in crystalline systems, a charge state DFT calculation and subsequent geometry relaxation was performed for each defect and the charge transition levels were calculated. Interestingly, due to the inherent randomness of the amorphous network, this results in a probability distribution function (PDF) of transition levels (Fig. 8.8). When these distributions are used in the meso-scale dielectric charging model (see Section 8.1), model predictions match experimental charging measurements (Fig. 8.3) more closely than our single trap-depth model from Year 2.

![Fig. 8.5: Comparison of the predicted densities of amorphous structures to experiment for $a$-SiO$_2$. MD/DFT were used for the predictions.](image)

![Fig. 8.6: Comparison radial distribution functions (RDFs) of MD/DFT predicted amorphous structures to experiment for $a$-SiO$_2$ and $a$-Si$_3$N$_4$.](image)
Electro-mechanical dielectric degradation associated with the hard landing of movable electrode is a technology-inhibiting reliability concern for capacitive RF-MEMS switches. In this contribution, we proposed two schemes for dynamic soft-landing of capacitive RF-MEMS switches that obviate the need for external feedback circuitry. Instead, the resistive and capacitive braking schemes we proposed can reduce impact velocity significantly without compromising other performance characteristics like pull-in voltage and pull-in time. Resistive braking is achieved by inserting a resistance in series with the voltage source whereas capacitive braking requires patterning of the electrode or the dielectric. Our results have important implications for the design and optimization of reliability-aware electrostatically-actuated capacitive MEMS switches.

We know that the pull-in of a capacitive MEMS switch is achieved by applying a step potential $V$ between the electrodes $M_1$ and $M_2$ (Fig. 8.9 (a)). Assuming $M_1$ at rest at $y_0$ (Fig. 8.9(b), point A), a step...
voltage $V < V_P$ (the pull-in voltage) imparts an energy $E_{T1} = \frac{1}{2} C(y_0)V^2$ to the membrane (Fig. 8.9(b), point B). Electrode $M_1$ eventually comes to rest at the minimum (point $P_1$) of the total potential energy ($E$) landscape defined by the sum of electrostatic energy

$$E = \frac{1}{2} C(y)V^2,$$

with $V_c$ being the voltage across the capacitor and spring

$$\frac{1}{2} k(y - y_0)^2.$$

potential energies (blue solid line in Fig. 8.9(b)). The energy difference between $E_{T1}$ and $P_1$ is lost due to air-damping. For step voltage $V > V_P$, however, the energy of $M_1$ jumps to $E_{T2}$ and since the energy landscape this time (red solid line in Fig. 8.9(b)) does not have any minima, the ‘limiting point instability’ results in uninhibited acceleration of $M_1$ that is eventually brought to a hard-stop at $y=0$ (point $P_2$ in Fig. 8.9(b)) by slamming against the immovable dielectric. It is this kinetic energy dissipation

$$E_d = \frac{1}{2} m v_{\text{impact}}^2$$

(Fig. 8.9(b), from point D to $P_2$) at the $M_1$/dielectric interface that damages the dielectric. Fig. 8.9(c) shows the displacement ($y$) and velocity ($v$) of the electrode $M_1$ as a function of time ($t$) during pull-in.

Various research groups have used open and closed loop control techniques to reduce $v_{\text{impact}}$ or $E_d$ for individual and ensemble of MEMS switches. These techniques craft the input waveform so that $V(t)$ is reduced below $V_P$ as $M_1$ approaches the dielectric, thereby ensuring a softer landing. These external circuits add to the cost and the waveform developed for a nominal switch is often not optimal for an ensemble of switches (due to process variations) and the worst-case design inevitably compromises global performance.

Towards the goal of developing a self-corrective, cost-effective, and process variation-tolerant...
soft-landing scheme, we have proposed two techniques to reduce $v_{\text{impact}}$ during the pull-in transient of the switch. The first method involves resistive feedback/braking (see Fig. 8.10) so that part of $E_d$ is remotely dissipated in a resistor away from $M_1$/dielectric interface, whereas the second method relies on the patterning of either of $M_1$, $M_2$ or the dielectric (see Fig. 8.11) in such a way that the effective capacitor area decreases dynamically as $M_1$ approaches the dielectric. Both the methods reduce $v_{\text{impact}}$ without compromising $V_{\text{PI}}$ and $t_{\text{PI}}$ significantly. The resistive braking concept was experimentally verified and a patent has been filed. We are seeking to validate capacitive braking in collaboration with Prof. Peroulis’s group.

8.3 Meso-scale Contact Model

During the reporting period we completed the development of a first principles-based meso-scale contact model that explicitly captures surface roughness effects and is parameterized from MD and ab initio simulations. The meso-scale model computes long-range (van der Waals) attractive interaction between the two surfaces that depend on the nature of the materials, given by the Hamaker constant and the roughness and the repulsive interaction resulting from the contacts. The attractive interactions are given by:

$$F_{\text{vdw}} = -A \sum_{i,j} \frac{\Delta L^2}{6\pi(z_{ij} + \bar{h})^3}$$

where $A$ is the Hamaker constant, $i$ and $j$ index the nodes used to sample the surface with height denoted by $z_{ij}$; $\bar{h}$ is the mean separation between the two surfaces. To compute the contact force we identify individual contacting regions and use an elasto-plastic relationship:

$$f_i(h) = \begin{cases} 
\frac{2}{3} E^* \sqrt{R_i \delta_i^3} & \text{for } \frac{2}{3} E^* \sqrt{R_i \delta_i^3} < H(A_i) \cdot A_i \\
H(A_i) \cdot A_i & \text{otherwise}
\end{cases}$$

where the first line represents the elastic interactions using a Hertz model ($E^*$ is an effective elastic constant, $R_i$ is the radius of curvature of the asperity, and $\delta$ is the local surface penetration) and the second line represents the plastic regime. $H(A_i)$ is the size-dependent hardness of the contact and $A_i$ is its area.

Figure 8.12 shows the contact force predicted by the model as a function of contact separation together with the elastic and electrostatic force from which the equilibrium separation between the two surfaces is

![AFM scan of PRISM dielectric surface roughness used in mesoscale contact model](a)

![Static force balance on membrane showing equilibrium contact distance](b)

Fig. 8.12: (a) AFM scan of PRISM dielectric surface roughness used in mesoscale contact model, and (b) static force balance on membrane showing equilibrium contact distance.
obtained. The force-displacement obtained from the mesoscale model is used in the device-level simulations and the mesoscale model is parameterized from the MD and DFT simulations described below.

8.3.1 Atomistic Simulations of Single-Asperity Contact

We characterize the mechanical response resulting from the metal (Ti)-dielectric (Si$_3$N$_4$) contact by using atomistic molecular dynamic simulation. When two rough surfaces are brought into contact, nanosize asperities form individual contacts that are initially deformed elastically until the local stress reaches the contact’s hardness and then, plastic deformation occurs. The systems of interest consist of Ti metal with an amorphous oxide layer (TiO$_2$) making contact with an amorphous silicon nitride (Si$_3$N$_4$) layer with an amorphous oxide layer (SiO$_2$) on top of it, as illustrated in Fig. 8.13 (a). A modified BMK potential is utilized for amorphous TiO$_2$, SiO$_2$ and Si$_3$N$_4$ and the EAM potential is used for Ti metal. Hardness is obtained from our MD simulations from the applied force and actual contact area when plastic deformation is observed:

$$\frac{H(A)}{A_{\text{contact}}} = \frac{F_{\text{closing}}}{A_{\text{contact}}}$$

where $F_{\text{closing}}$ is the closing force and $A_{\text{contact}}$ is for the effective contact area. We use various asperity sizes by controlling the asperity height and peak-to-peak distance. The strength of the contact is determined by the stress that is required to break the contact.

Figure 8.13 (b) shows the contact stress as a function of contact size as the load on a single contact is increased. The circles mark the initiation of plastic deformation and the size-dependent hardness of the materials used in the meso-scale contact model. We obtained the hardness of the contact as a function of contact size with various asperity heights and contacting structure. The strength of the contacts is the stress needed to open the contact and is important in contact adhesion. Contact strength is also strongly size-dependent. Our simulations show significant strengthening of the contacts as the size decreases. This is consistent with the general observation that “smaller is stronger”.

Fig. 8.13: (a) Schematic of nanoscale metal-dielectric contact, and (b) contact stress as a function of contact size. The black circles mark plastic deformation and indicate size-dependent hardness.
8.4 Multiscale Micromechanical Models

8.4.1 Atomistically-Informed Dislocation Dynamics

During Year 3, we incorporated deformation mechanisms at atomic scales into a phase field mechanical models (PFMM) code. PFMM is a 3D parallel code and has shown good scalability on more than 2000 processors and datasets with over 8 billion degrees of freedom. Deformation mechanisms in nanocrystalline metals have been the focus of extended discussion, especially since molecular dynamics simulations have been able to reveal possible mechanisms at atomistic scales, such as grain boundary accommodation, dislocation emission and absorption at grain boundaries and twinning also observed in experiments. Understanding the mechanical behavior at this scale is fundamental for ensuring reliability prediction of structures with components constituted of nanocrystalline materials, such as MEMS (micro-electro-mechanical-systems). Molecular dynamics simulations show that with grain sizes in the nanometer scale, plastic deformation is mostly driven by the emission and absorption of partial dislocations at the grain boundaries. In nanocrystalline metals, the emission of partial dislocations from the grain boundaries is the driving mechanism of plastic deformation for Ni and Cu, while for Al perfect dislocations are also observed. Therefore, incorporating partial dislocations is of critical importance in simulating the mechanical behavior of nanocrystalline Ni. During Year 3, we included partial dislocations in the PFMM code. The simulations show a inverse relationship between the stacking fault energy and the equilibrium stacking fault width shown in Fig. 8.14. Furthermore, our results show that the equilibrium configurations cannot be described only by the ratio between the intrinsic and unstable stacking fault energies as previously suggested, but rather by their product. Details of this work may be found in Ref. 97.

We have studied the relation between the core energy and the dislocation mobility with a first principles-based, multiscale single crystal plasticity model for fcc metals and have applied it to nickel. The model consists of the PFMM with all its input parameters obtained from equilibrium and non-equilibrium molecular dynamics (MD) simulations. The atomistic information used to inform the phase field model includes: elastic constants, dislocation core energy, crystal disregistry energy (gamma surface), and dislocation mobility. The PFMM model can be simplified to the Frenkel-Kontorowa equations for straight dislocations and under these conditions, an analytical time-dependent solution enables a direct connection to non-equilibrium MD simulations. Our simulations show that decreasing the stacking fault energy increases the dislocation mobility. These results have recently been published in Ref. 98.

8.4.2 UQ of Yield Stress Prediction

The Hall-Petch relation for polycrystals in which the strength increases as the grain size is reduced can be derived using a model of dislocation pile ups. As the grain size decreases below 20-40 nm, the inverse Hall Petch relation is observed, which manifests as softening for smaller grain sizes. To capture this transition, both dislocation interactions and grain boundary deformation should be taken into consideration. In a recent paper, Koslowski, Lee and Lei were able to predict the relation between...
grain size and grain boundary energetics and the strength of nanocrystalline nickel. The maximum strength depends not only on the average grain size but also on the grain boundary energetics. On the other hand, for large grain size (above 100 nm) experimental results show good agreement with the Hall-Petch relation, while for smaller grain size the yield stress shows a large scatter in the data.¹⁰¹ We carry out PFMM simulations to quantify the uncertainty in the strength of polycrystalline nickel due to uncertainties in the grain size distribution. The grain size distribution is obtained from TEM measurements in Professor Stach’s group. Figure 8.15 shows the yield stress calculated with our simulations with uniform and bimodal grain distribution. The yield stress is defined with the 0.1% offset (black) and 0.2% offset (red) for comparison. For grain sizes below 20 nm the difference in the yield stress due to the grain size distributions can reach up to 20%.

The uncertainty in the yield stress of the nanocrystalline membrane in the PRISM device is calculated as follows. The yield stress as a function of the grain size is calculated with PFMM simulations for uniform and bimodal grain size distribution in the range 4 to 130 nm. We propagate the PDF of grain size distribution to calculate the PDF of the yield stress. The results are shown in Fig. 8.16. The solid line corresponds to the yield stress calculated with the PFMM uniform grain size distribution and the dashed line corresponds to a bimodal grain distribution. The uncertainty in the grain size distribution is reflected in an uncertainty in the yield stress of 10%.

```
fig 8.15: Predicted yield stress as a function of grain size. Solid symbols correspond to uniform grain distribution, open symbols are non uniform grain size.
```

```
fig 8.16: Propagation of PDF of grain size to PDF of yield stress. The grain size distribution changes with the height (a) 75 nm (b) 365 nm (c) 890 nm (d) 1250 nm.
```
8.5 Constitutive Modeling of PRISM Membrane Plasticity

During Year 3, development of constitutive models in MEMOSA-MPM was continued and several key extensions were completed. MEMOSA-MPM now has several choices for constitutive models beyond the isotropic, linear elastic model with which we began. An algorithm has been implemented and tested for anisotropic elasticity. The algorithm rotates strain increments to the material frame, computes a stress increment in that frame and then rotates the result back to the laboratory frame. The orientation of the material frame relative to the laboratory frame is encoded using Euler angles to represent the rotation.

We also implemented and tested a von Mises (J2) plasticity model with linear isotropic hardening in MEMOSA-MPM. Moreover, we have implemented a single-crystal plasticity model and tested the implementation with a driver code. This year we continued development of a J2 plasticity model for polycrystals that includes size effects. The goal is to develop a homogenized model that describes the effective mechanical response of the thin Ni film found in the PRISM device. As a basis, we use the single-crystal plasticity model with size effects of Ref. 102. The J2 model was developed by averaging material properties over all grains along the film thickness in that model. The rate-independent version of this J2 model is summarized as follows.

\[
\sigma = E : \varepsilon' \quad \text{where} \quad \varepsilon = \varepsilon' + \varepsilon''.
\]

The yield criterion is based on the J2 stress, \( \bar{\sigma} = \left( \frac{3}{2} \sigma^d : \sigma^d \right)^{\frac{1}{2}} \) with \( \sigma^d \) being the deviatoric part of the stress tensor. Specifically, the yield function is \( f(\sigma, \tau^c) = \bar{\sigma} - \tau^c(\gamma) \), where \( \tau^c(\gamma) \) describes the hardening inspired by an effective critical resolved shear stress from the single crystal model. We use an associative flow rule for evolution of the plastic strain

\[
\varepsilon'^p = \dot{\gamma} \frac{\sigma^d}{\left( \sigma^d : \sigma^d \right)^{\frac{1}{2}}}
\]

The critical resolved shear stress evolves in the following way:

\[
\dot{\tau}^c = \frac{1}{2} A a \mu \left( \frac{\tau^0}{\tau^c} \right) \dot{\gamma}
\]

With the initial value \( \tau^c(0) = \sigma^\gamma \) being the initial yield strength of the material and where \( \tau^0 = A \sqrt{\mu b} \sqrt{\rho} \), \( \rho = 2 \rho_{sat} / h + \rho_0 \). The constants \( A \) and \( a \) are determined from micromechanical simulations, \( \mu \) is the shear modulus, \( b \) is the magnitude of the Burger’s vector for Ni, \( \rho \) is the dislocation density and \( h \) is the grain size. Finally, \( \rho_0 \) is the initial dislocation density and \( \rho_{sat} \) is the saturation value.

Size effects enter the model through the dependence of the initial yield stress on the grain size and through the dependence of the hardening on grain size.

This model has been implemented in MEMOSA-MPM. Using this implementation, we studied the mechanical response of a thin Ni film under uniaxial tensile stress. Results were compared with experimental data shown in Refs. 103 and 104. The values of the parameters used in the experiments are shown Table 8.1. The parameters \( A \) and \( a \) were, for now, chosen to fit data in Ref. 103. The sources for other parameters is also given in the table.
Figure 8.1 shows experimental tensile stress-strain curves for as-deposited LIGA Ni (4um grain size) and annealed Ni (40um grain size) microsamples from Hemker and Last. The initial yield stress is 410 MPa for the as-deposited sample and 120 MPa for the annealed sample. Figure 8.1 also shows experimental tensile stress-strain curves for different as-deposited LIGA Ni microsamples from Hemker and Sharpe. Curves with higher yield stress correspond to microsamples with smaller grains. The bottom curve corresponds to grain sizes of 4 µm and the curve below the one at the top corresponds to a grain size of 200 nm. The grain size and yield stress of the rest of the curves are not available. Values were estimated by eye and linear interpolation. From bottom to top, the second curve was assigned a grain size of 2.48 µm and a yield stress of 790 MPa. The third curve was assigned a grain size of 1.85 µm and a yield stress of 930 MPa. The fourth curve was given a yield stress of 1180 MPa. The fifth curve was assigned a grain size of 160 nm and a yield stress of 1280 MPa. Note that the plastic behavior shown from the model has an upward concavity, as opposed to the downward concavity shown in the experiments. We expect to improve behavior with a rate-dependent model.

Figure 8.17 shows experimental tensile stress-strain curves for as-deposited LIGA Ni (4um grain size) and annealed Ni (40um grain size) microsamples from Hemker and Last. The initial yield stress is 410 MPa for the as-deposited sample and 120 MPa for the annealed sample. Figure 8.17 also shows experimental tensile stress-strain curves for different as-deposited LIGA Ni microsamples from Hemker and Sharpe. Curves with higher yield stress correspond to microsamples with smaller grains. The bottom curve corresponds to grain sizes of 4 µm and the curve below the one at the top corresponds to a grain size of 200 nm. The grain size and yield stress of the rest of the curves are not available. Values were estimated by eye and linear interpolation. From bottom to top, the second curve was assigned a grain size of 2.48 µm and a yield stress of 790 MPa. The third curve was assigned a grain size of 1.85 µm and a yield stress of 930 MPa. The fourth curve was given a yield stress of 1180 MPa. The fifth curve was assigned a grain size of 160 nm and a yield stress of 1280 MPa. Note that the plastic behavior shown from the model has an upward concavity, as opposed to the downward concavity shown in the experiments. We expect to improve behavior with a rate-dependent model. Figure 8.18 shows numerical results obtained by the Koslowski group using PFMM. The computations consider tensile stress loading of nanocrystalline Ni. From bottom to top we have grain sizes of 16nm, 8nm and 4nm. The corresponding yield stress is 7.75GPa, 8.7GPa and 9.3GPa.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus</td>
<td>E</td>
<td>180 GPa</td>
<td>Hemker &amp; Last</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>ν</td>
<td>0.2</td>
<td>Rodney, et al.</td>
</tr>
<tr>
<td>Magnitude of Burger’s vector</td>
<td>b</td>
<td>2.5x10^-10 m</td>
<td>Rodney, et al.</td>
</tr>
<tr>
<td>Taylor parameter</td>
<td>a</td>
<td>0.3</td>
<td></td>
</tr>
<tr>
<td>Initial dislocation density</td>
<td>ρ₀</td>
<td>10¹⁸ m⁻²</td>
<td>Hunter, et al.</td>
</tr>
<tr>
<td>Saturation dislocation density</td>
<td>ρ sat</td>
<td>4.07 m⁻²</td>
<td>Hunter, et al.</td>
</tr>
<tr>
<td>Matrix row sum</td>
<td>A</td>
<td>7.6x10⁻²</td>
<td></td>
</tr>
</tbody>
</table>

Table 8.1: Parameters for J2 model
The compact model of gas damping developed in Years 1 and 2 and those available in the literature have been based on small-displacement motion of microbeams. Because of the importance of damping in determining the impact velocity at contact, a new near-contact damping model was developed for application in the coarse-grained model of the PRISM device.

Gas damping simulations were performed with the quasi-steady ES-BGK solver at various beam-to-substrate gap heights. The geometric parameters correspond to the silicon cantilever beams of an inertial g-switch designed to actuate at very high acceleration levels (10,000 to 50,000 g). Figure 8.19 shows a micrograph of the switch and a schematic of the computational domain for the damping simulations. The computed variation of the damping force during the accelerometer beam actuation is then used in beam dynamics models to predict the time for switch closing and opening. These are measured experimentally for various acceleration profiles and compared with modeling. The use of inertially-actuated microbeams allows us to isolate possible effects of air and solid dielectric charging on dynamics of the microbeam.

Typical ES-BGK simulation results for the gas flow around the moving accelerometer beam are shown in Fig. 8.20. Figure 8.20(a) shows the pressure and flow fields around the beam for two air gap values, 0.1 and 1 micron. The corresponding air velocity magnitudes are shown in Fig. 8.20(b). Note that the beam in both cases is moving downward with a velocity of 0.1 m/s. The flow fields are typical for a squeeze film damping when the gas is being pushed out from a narrow gap between parallel surfaces in relative out-of-plane motion. The air velocity field has a vortical structure around the edge of the beam. This is generated by a jet of air that emanates from the beam-to-substrate gap. Note that the jet velocity is higher than that of the beam for the small gaps of the accelerometer beams. The contours in Fig. 8.20(b) show a gas jet
emanating from the gap with speeds that are ~50% higher than the beam velocity itself.

The pressure difference between the bottom and top of the beam leads to the air damping force that opposes the beam motion. The origin and magnitude of such force is illustrated by the normal pressure component on the bottom of the beam which is shown in Fig. 8.21(a). It can be seen that the pressure at the bottom of the beam is about 10% above atmospheric for 0.1 micron, whereas it is about 2% above for 1 micron gap. The increase in the maximum pressure is about 5 times higher for the 0.1 micron gap as compared to that at 1 micron and points to a slower than linear dependence of the damping coefficient on the gap size as it approaches zero. Though the beam velocity itself remains the same for the two cases, the smaller gap leads to a much higher pressure at the bottom surface of the beam leading to a much higher damping.

The ES-BGK simulations were performed for various gap sizes ranging from about 50 nm to 2 μm. The 50 nm lower limit is the estimated effective gap when the beam bottom surface contacts the substrate due to finite asperities on both surfaces. Note that the gap between two atomically rough surfaces never goes to zero due to a finite surface roughness. The computed variation of the gas damping coefficient as a function of gap size obtained using the ES-BGK simulations is shown in Fig. 8.21(b). Also shown are earlier models from literature. In particular, the thin-beam model \(^{105}\) is also based on ES-BGK simulations but for beam geometries that have width-to-beam ratio of 10 and higher. The model of Gallis and Torcynzski model \(^{106}\) is obtained also for relatively thin beams and using a Reynolds equation with modified boundary conditions. While the Gallis-Torcynzski model and the simulations performed in
this work agree well for the larger gap sizes, there is significant discrepancy for the smaller gaps. This is largely due to the fact that the Gallis-Torcynzski model was developed based on simulations performed for a certain range of gap sizes and is not valid for very small gaps in the near-contact regime. The thin-beam model leads to significant over-prediction of the damping coefficient for all gap sizes because it assumes a linear dependence on the beam thickness. It can be clearly seen that the Gallis-Torcynzski model leads to infinite damping at very small gaps as opposed to the simulations performed here, which predict a finite damping even for a gap size of 50 nm.

These differences are reflected in Fig. 8.22, which shows a comparison between experimental values of switch closing time and that computed using the different models. Our new model correctly captures experimental trends. The previously published models were developed mostly for non-contacting beam oscillation dynamics. The comparison underlines the importance of correctly accounting for the conditions specific to near-contact damping occurring in RF MEMS switches and other contacting microsystems.

8.7 Modal-Analysis Based Model for Switch Dynamics with Uncertainty Quantification

In the third year of this effort, a computationally-tractable reduced-order model for PRISM switch dynamics was extended to address realistic switch geometries. The extensions included beam curvature and realistic end boundary conditions employing an analytical model for torsional springs (see Fig. 8.23). This model retains the most pertinent multi-physics phenomena necessary for switch analysis, including initial curvature, residual stress, electrostatics, and a compact model for fringing-field effects and squeeze-film damping. The model also accounts for the effects of Knudsen number, and the interaction of the beam with the dielectric layer on the electrode with which it contacts and impacts as it pulls in. The equation governing the motion is given by:

\[
\frac{\partial^4 \dot{w}}{\partial \hat{x}^4} + \frac{\partial^2 \dot{w}}{\partial \hat{t}^2} + c(\hat{w})\frac{\partial \hat{w}}{\partial \hat{t}} = \alpha_1 \int_0^1 \frac{\partial \dot{w}^2}{\partial \hat{x}} - 2\frac{\partial \dot{\hat{v}}}{\partial \hat{x}} \frac{\partial \dot{w}}{\partial \hat{x}} d\hat{x} \left( \frac{\partial^2 \dot{w}}{\partial \hat{x}^2} - \frac{\partial^2 \hat{v}}{\partial \hat{x}^2} \right) + N \frac{\partial^2 \hat{w}}{\partial \hat{x}^2} + \frac{\alpha_2 V^2(t)}{(1 + \hat{v} - \dot{\hat{w}})^2} (1 + A_1 (1 + \hat{v} - \dot{\hat{w}})^{0.76}) (H(\hat{x} - \hat{x}_1) - H(\hat{x} - \hat{x}_2)) + \alpha_3 (\hat{w} \geq \frac{g_0 - t_{air}}{g_0} \dot{\hat{w}} + \hat{v}) (\dot{w} - \frac{g_0 - t_{air}}{g_0} + \dot{\hat{w}}),
\]

where \( v(x) \) is the initial curved beam, \( w(x,t) \) is the deflection from the initial configuration, \( N \) is the residual stress/force along the beam, \( c(w) \) is an appropriate correction for squeeze film damping, and \( A_1 \) is a fringing-field correction.
It is assumed that the solution to the above equation can be approximated by a linear combination of the first \(M\) linear modes of the undamped straight beam. The solution then takes the form

\[
\hat{w}(x,t) = \sum_{i=1}^{M} u_i(t)\phi_i(x)
\]

where \(\phi_i\) is the \(i\)-th linear undamped mode of the beam with appropriate boundary conditions and \(u_i\) are time varying coefficients. The mode shapes are the solutions to the equation:

\[
\phi''_i = N\phi''_i + \omega_i^2 \phi_i
\]

with appropriate boundary conditions. The initial curve for the beam is also assumed to be represented by a Fourier approximation:

\[
v(x) \approx \sum_{i=1}^{M} p_i \sin(\pi x)
\]

Fig. 8.23: Geometry and nomenclature for curved beam model.

Now applying the modal expansion and following the usual order reduction process, the final equations in modal amplitudes are:

\[
\ddot{u}_n + \omega_n^2 u_n = \int_0^1 c(w) \hat{w} \phi_n dx + \\
\alpha_1 \sum_{i,j,k=1}^{M} u_i u_j u_k \int_0^1 \phi'_i \phi'_j dx \int_0^1 \phi''_k \phi_n dx + \\
\alpha_1 \sum_{i,j,k=1}^{M} u_i p_j u_k \int_0^1 \pi j \phi'_i \cos(x \pi j) dx \int_0^1 \phi''_k \phi_n dx + \\
\alpha_1 \sum_{i,j,k=1}^{M} u_i u_j p_k \int_0^1 \phi'_i \phi'_j dx \int_0^1 -\pi^2 k^2 \sin(x \pi k) \phi_n dx + \\
\alpha_1 \sum_{i,j,k=1}^{M} u_i p_j p_k \int_0^1 \pi j \phi'_i \cos(x \pi j) dx \int_0^1 -\pi^2 k^2 \sin(x \pi k) \phi_n dx + \\
\alpha_2 V(t)^2 \int_{x_1}^{x_2} \left( \frac{1}{(1 + v - w)^2} + \frac{A_1}{(1 + v - w)^{1.24}} \right) dx + \\
\alpha_3 \int_0^1 (w - v - t_{air})(w \geq v + t_{air}) dx,
\]

\(n = 1...M\).
This model of the curved switch was extensively used to study the effects of model parameters on the important switch performance variables including static and dynamic pull-in voltages, and switch closing as well as opening times. To compute these performance measures, numerical techniques needed to be developed to find solutions of the highly nonlinear models in the above equation.

Using the model above, the effects of input parameter variations on system performance were also investigated for a few representative realistic situations. The analysis was restricted to parameter variations with normal distributions. For UQ analysis, the three quantities of interest are the static pull-in voltage, the dynamic pull-in voltage, and the switch closing time. The static pull-in voltage is defined as the highest voltage at which there exists at least one equilibrium solution to the system not involving contact. The static solutions were found via an enforced displacement scheme. In contrast, the dynamic pull-in voltage is defined as the amplitude of a step voltage applied to the system that causes it to close. This voltage is smaller than the static pull-in voltage due to dynamic effects, typically by 8% or so, but this can vary based on switch geometry. The dynamic pull-in voltage is found via a bisection search method.

For the response surface generation, a straightforward Latin Hypercube sampling was implemented. The response surfaces were generated using multi-variate adaptive regression splines (MARS). The geometry was chosen corresponding to a Gen 2 PRISM switch. The centerline curve of the switch is shown in Figure 8.24. The nominal geometric and material parameters for the curved switch are: L=395 μm (std. dev 3.25), b=121.8 μm (std. dev 1.36), h=3.97 μm (std. dev 0.59), t_{air} = 2.5 μm (std. dev 0.15), t_{d}=0.28 μm (std. dev 25 nm), x_{1}=0.3 (std. dev=0.004), x_{2} = 0.7 (std. dev. 0.004), E=170 GPa (std. dev. 7), ν=0.31 (std. dev. =0.005) , σ=0 MPa (std. dev 3), ρ = 8900 kgm^{-3} (std. dev 100 kgm^{-3}), p_{1} = 1.161 μm (std. dev 0.3 μm).

Since the model depends on more than 20 parameters, a linear sensitivity analysis was conducted around the nominal parameter values to determine the most critical parameters that were found to be L, h, t_{air}, E, σ and p. The response surfaces for this case were generated from 400 sample points. K-fold cross-validation resulted in an averaged $R^2$ of greater than 0.999. Example response surfaces are shown in Fig. 8.25.
Given these data, to develop smooth PDFs of pull-in voltage and closing time, $10^6$ Monte Carlo samples were generated for un-correlated as well as correlated parameters. The resulting histograms of results are given in Fig. 8.26. The most critical parameters were found using a local sensitivity analysis, and they are the switch thickness, air gap height, and first Fourier coefficient of the initial beam curvature. This is because the system is very sensitive to these dimensions and vertical dimensions are typically among the most difficult to control.

Fig. 8.26: Histograms of static pull-in voltage and switch closing time for un-correlated parameters.
9. ENHANCEMENTS TO NUMERICAL METHODS AND SOFTWARE

9.1 Adaptive Collocation in MEMOSA-UQ

During Year 2, significant resources were devoted to developing a user-friendly Python-based software framework for uncertainty quantification called MEMOSA-UQ. The central focus was on collocation-based gPC for uncertainty propagation (see Fig. 9.1). The analysis is driven by a set of input parameters, each characterized by a probability density function (PDF). Parameters can be specified with a mean and standard deviation for a Gaussian distribution, or with a set of discrete values for an experimentally-obtained PDF. These parameters are fed to a Sweep object, which implements Smolyak sparse grid sampling, Latin Hypercube sampling, or random Monte Carlo sampling. The sweep is connected to a Host object, which manages a series of executions. The InteractiveHost runs jobs on the local machine, while a PBSHost sends them off to the Portable Batch System (PBS) on a remote host. The underlying model code can be written in Python or in any other language; specific parameter values for each run are passed via the command line. Results are stored in an HDF5 format file, with proper metadata to characterize the experiment and all results. The framework also builds an overall response surface and computes PDFs for designated output values.

During Year 3, a number of enhancements were made to MEMOSA-UQ. We took Agarwal and Aluru's work on domain adaptive stochastic collocation and integrated it into our UQ framework. This scheme adaptively decomposes the random domain into sub-domains, sampling more points where the output changes rapidly. This makes it useful for models with discontinuities or rapidly-changing output, such as the switch displacement for voltages around pull-in or pull-out. A number of improvements were made to the workflow to improve performance. In the current implementation, MEMOSA-UQ caches all previous results, preventing the running of duplicate simulations, thus decreasing the time for UQ runs to almost half. MEMOSA-UQ also allows us to take the output from a previous UQ run and refine it, using the previous results, and creating new sub-domains where necessary.

With all of its UQ methods, MEMOSA-UQ provides for plotting of probability density functions (PDFs) and response surfaces. For the adaptive work, it can also plot scatter graphs showing the refinement in the output for each iteration (Fig. 9.2). Also, like the Smolyak method, users can easily apply different input PDFs to previous UQ runs. The computed response surface (made up of all the sub-domains) is used to quickly compute the new output PDF.

![Fig. 9.1: MEMOSA uncertainty quantification software environment](image-url)
9.2 Compact Model Database in MEMOSA-UQ

During Year 3, work on the design and implementation of a workflow for Bayesian network UQ analysis at the system level was initiated. A central component of the implementation is a compact model database to store response surfaces corresponding to the “model” nodes in Fig. 2.6. In addition, information about inputs to the models is also stored in the database. This includes experimental PDFs as well as PDFs computed using simulations. Furthermore, MEMOSA-UQ provides a GUI to access the database.

The overall workflow takes the following form: first, we estimate input parameters for our simulations, using worst-case minimum and maximum values with uniform distributions. Then we run the simulations (which may take weeks for complex simulations). The resulting response surfaces are added to the compact model database. Using either experimental, estimated, or computed PDFs, the output of the response surfaces may be computed; these, in turn, form inputs to other models in the Bayesian network in Fig. 2.6. Models and inputs may be changed by the user as more data and better models become available.

The database is hosted online and access to it is through a web-based interface. The workflow manager is designed to assist the researcher to identify the correct model (response surface) and the input PDFs with which compose the Bayes network. For example, if a response surface needs a Young's modulus PDF as an input, the database is searchable to identify the Young's modulus for the material of interest. An early prototype of the GUI to access the compact model database is shown in Fig. 9.3. Work is underway to refine and develop the MEMOSA-UQ platform for calibration and system-level UQ, and progress will be reported in due course.

Fig. 9.2: Sample output from adaptive UQ computation showing adaptively-placed collocation points.

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9.3 Enhancements to MEMOSA-FVM

A number of enhancements were made to MEMOSA-FVM during Year 3. These include, among others: (i) the development of a plate element model to speed up the computation of high aspect ratio membranes, and its integration in the immersed boundary framework to enable fluid-structure-electrostatics computations; (ii) the development of a creep model, and its integration with the full elastic stress analysis formulation in MEMOSA-FVM, as well as with the plate element model; (iii) the development of a residual stress model in conjunction with stress analysis; (iv) completion of the ES-BGK implementation in the unstructured finite volume formulation of MEMOSA-FVM; and (v) enhancements to scaling. Here we focus on a few key enhancements critical to project goals.

9.3.1 Plate Element Model

In order to keep actuation voltages low enough to control dielectric charging, RF-MEMS switches are frequently fabricated with extremely thin membranes, frequently no more than 1-3 μm thick. Given membrane lengths of 400-500 μm, membrane aspect ratios of 100-500 may result, leading to very stiff linear systems and slow convergence of numerical solutions. In the limit of very thin plates, Mindlin-Reissner plate elements offer an efficient alternative to the complete solution of the 3D elasticity equations in the membrane. During Year 3, we developed a finite volume framework for Mindlin-

Fig. 9.3: A prototype of the GUI for the compact model database.

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Reissner plate elements, implemented the scheme in MEMOSA-FVM, tested and verified it against the complete elasticity solution in the thin-plate limit, and used it for prediction of pull-in, contact, and pull-out. Details may be found in Ref. 107.

A variety of verification problems were computed to establish the correctness of the plate element formulation and implementation. The temporal accuracy of the plate element model is tested by studying the undamped vibration of a thin fixed-fixed plate subjected to a uniformly distributed load. If the Poisson’s ratio is set to be zero, then the transient deflection of the plate will be given by Euler-Bernoulli beam theory, and the natural frequency \( \Omega \) may be derived as:

\[
\Omega = 1.03 \sqrt{\frac{E}{\rho L^2}} h
\]

where \( L \) =400 \( \mu \)m is the length, \( h \)=2\( \mu \)m is the thickness, \( E \) is the Young’s modulus, and \( \rho \) is the density of the plate. Young’s modulus and the density of the plate are taken to be \( E = 200 \) GPa and \( \rho = 7854 \) Kg/m\(^3\) respectively. The natural frequency is calculated to be \( \Omega = 6.497 \times 10^4 \) Hz. To simulate this problem, the plate is assumed to have \( u = 0 \) and \( \frac{\partial u}{\partial t} = 0 \) as the initial conditions. At time \( t = 0 \), an uniform load is applied on the plate. This causes the plate to vibrate in a sinusoidal motion. A 40x40 mesh is used for this problem based on a mesh convergence study. The time-step in this problem is taken to be \( \Delta t = 10^{-5} \) seconds. The results of the plate element model for the mean deflection at the plate center and the natural frequency are compared with the analytical solution in Table 9.1. It is seen that the numerical results are within 0.2% of the analytical results.

The plate element model was also used to compute the pull-in voltage of the PRISM RF-MEMS switch. The main dimensions of the membrane are length \( L=400 \) \( \mu \)m, width \( b = 100 \) \( \mu \)m and thickness \( h = 4 \) \( \mu \)m. The predicted maximum deflection at the center of the membrane is compared with that obtained using the structural solver in MEMOSA-FVM in Fig. 9.4 as a function of the applied voltage. The results obtained with the MEMOSA-FVM structural solver are based on a 2D finite volume solution using the complete linear elastic constitutive equations.

Two cases are considered: in Case (a), in which the length of the pull-down electrode is the same as that of the membrane, and Case (b), in which the pull-down electrode has a length of 80 \( \mu \)m centered about the centerline of the membrane. To make comparison with those results, Poisson’s ratio in the present simulation is set as \( \nu = 0 \). It is

<table>
<thead>
<tr>
<th>Method</th>
<th>Mean Plate Deflection (( \mu )m)</th>
<th>Natural Frequency (Hz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analytical</td>
<td>(-5.0 \times 10^{-5})</td>
<td>(6.497 \times 10^4)</td>
</tr>
<tr>
<td>FVM</td>
<td>(-4.99 \times 10^{-4})</td>
<td>(6.485 \times 10^4)</td>
</tr>
</tbody>
</table>

Table 9.1: Comparison of mean plate deflection and natural frequency for undamped vibration of a fixed-fixed plate using plate element model.

Fig. 9.4: Maximum deflection of RF-MEMS switch under static pull-in. Case (a) refers to the case when the electrode is the same length as the membrane, while in Case (b), the electrode is 80 \( \mu \)m long. The structural model corresponds to a full linear elasticity solution for the membrane while the plate model employs plate elements based on Mindlin-Reissner plate theory.
seen that the deformation at the plate center obtained with the plate element model compares reasonably well with that obtained with the structural solver. However, it is seen that the plate element model slightly overestimates the pull-in voltage. The pull-in voltages obtained with the in-house structural solver are 181 V and 270 V for Case (a) and Case (b) respectively, whereas those obtained with the plate model are 187 V and 273 V respectively. Thus the pull-in voltages obtained with the plate model are higher by around 3.3% than those obtained with the structural solver. The difference may be attributed to non-linear stretching effects which are absent in the current plate model. Non-linear stretching increases the deformation rate and decreases the pull-in voltage. The larger pull-in voltage for the partial bottom electrode case can be explained by the fact that the electrostatic force is applied only over the middle region of the membrane. Thus a larger force is necessary for deforming the top electrode, which results in a higher pull-in voltage. The dynamic pull-in voltage for the case when both of the electrodes have the same length is found to be 171 V. Thus the dynamic pull-in voltage is less than the corresponding quasi-static pull-in voltage by around 9%. This result is similar to what has been reported in Refs. 108 and 109.

9.3.2 Creep Model in MEMOSA-FVM
During Year 3, MEMOSA-FVM was enhanced to model creep and visco-plasticity, both in the full structural solver and in the plate element model described above. In this framework, the strain tensor $\varepsilon$ is assumed to be the sum of elastic $\varepsilon^e$ and visco-plastic $\varepsilon^{vp}$ component:

$$\varepsilon = \frac{1}{2} \left[ \nabla \mathbf{w} + (\nabla \mathbf{w})^T \right] = \varepsilon^e + \varepsilon^{vp}$$

Here, $\mathbf{w}$ is the displacement vector. The stress tensor is related to the strain tensor $\varepsilon$ as follows:

$$\sigma = 2\mu (\varepsilon - \varepsilon^{vp}) + \lambda \text{tr}(\varepsilon - \varepsilon^{vp}) \mathbf{I}$$

In the above equation, $\mathbf{I}$ is the unit tensor, $\mu$ and $\lambda$ are Lamé coefficients. The equation governing the motion of an elastic-viscoplastic solid is:

$$\frac{\partial^2 (\rho \mathbf{w})}{\partial t^2} - \nabla \cdot \left[ \mu \nabla \mathbf{w} + \mu (\nabla \mathbf{w})^T + \lambda \text{tr}(\nabla \mathbf{w}) \right] = \rho \mathbf{f} - \nabla \cdot \left[ 2\mu \varepsilon^{vp} + \lambda \text{tr}(\varepsilon^{vp}) \right]$$

The typical creep curve, as shown in Fig. 9.5, has three stages. The transient stage I, referred to as primary creep, is characterized by decreasing creep rate. The second linear region II is the steady-state or secondary creep, and has constant strain rate. This region lasts longest, and is therefore most important for lifetime predictions. The third stage III, also known as tertiary creep, is characterized by rapid increase in strain-rate eventually leading to rupture.

A large number of constitutive models have been developed for estimating the steady-state creep under different conditions, including power-law creep, Coble creep, Nabarro-Herring creep, dislocation glide, and grain boundary sliding. At any applied stress, the steady-state creep rate can be expressed as:

$$\dot{\varepsilon}_c \propto \left( \frac{\sigma}{G} \right)^m$$

where $\dot{\varepsilon}_c$ is the creep strain-rate, $G$ is the shear modulus, and $m$ is the creep stress exponent. Different creep mechanisms can be identified with different values of $m$: diffusion creep is characterized by a linear
stress and strain-rate relationship, grain boundary sliding is characterized by \( m = 2 \), and power-law creep is characterized by \( m > 3 \). The creep strain-rate may be expressed in the form:

\[
\dot{\varepsilon}_c = A_c \left( \frac{\sigma}{\sigma_y} \right)^m
\]

where \( A_c \) is a material dependent constant. We assume strain-hardening of the form:

\[
\sigma_y = \sigma_{y0} \left[ 1 + B \left( \varepsilon_c^{\text{eff}} \right)^n \right]
\]

Here \( \varepsilon_c^{\text{eff}} \) is the effective or von Mises part of creep strain, and \( \sigma_{y0} \) is the initial yield stress. We present one representative verification test below. A complete description of the underlying numerical method and associated verification exercises may be found in Ref. 113.

In this test, MEMOSA-FVM is used to study the long-term creep deformation of fixed-fixed membranes. The computation is conducted using the complete structural solver as well as the plate element model; for high-enough aspect ratios, the two are expected to yield nearly identical solutions. In this test, a fixed-fixed beam is subjected to a distributed load, as shown in Fig. 9.6. Young’s modulus, Poisson’s ratio, and the density of the material are taken to be \( E = 200 \) GPa, \( \nu = 0 \), and \( \rho = 7854 \) Kg/m\(^3\) respectively. A 20x1000 mesh is used for this simulation, based on a mesh-convergence study. The top surface of the beam is assumed to be traction-free, and the left and right faces are constrained to have zero displacement. A distributed load of \( w = -10^4 \) Pa is applied on the bottom face. The beam instantaneously develops an elastic deformation, described well by Euler-Bernoulli beam theory. The deformation increases with time as creep sets in. For this test, the creep strain rate in the beam is determined using

\[
\dot{\varepsilon}_c = A_c \left( \frac{\sigma}{\sigma_y} \right)^m
\]

The relevant creep parameters used in the simulation are \( A_c = 8.33 \times 10^6 \)s, \( B = 1.8 \times 10^8 \), \( m = 2 \), \( n = 2 \), and \( \sigma_{y0} = 1 \) GPa. A time-step of \( \Delta t = 1 \) hr is used in the simulation. Contours of elastic strain and creep strain after 500 hrs are shown in Fig. 9.7 using the full structural solver. It is seen that after 500 hrs, the plastic strain in the device is of the same order of magnitude as the elastic strain. Creep simulations are also performed using the plate element model based on Mindlin-Reissner plate theory. In this simulation, a thin fixed-fixed plate with dimensions of 400 \( \mu \)m x 100 \( \mu \)m x 4 \( \mu \)m is simulated. The plate has same Young’s modulus and Poisson’s ratio as the 2D fixed-fixed beam. The temporal variation of the total and plastic deflection at the beam center obtained with the full structural solver is compared with the deflection at the plate center obtained with the plate model in Figs. 9.8(a) and (b). It is seen that deflection obtained with the complete structural solver is well within 1% of that obtained with the plate model after 500 hours.
Residual stresses play a critical role in determining membrane deformation in the RF-MEMS switch. Thus far, we have modeled the effects of residual stress in the PRISM device by employing an effective Young’s modulus. During Year 3, we introduced a residual stress term in MEMOSA-FVM’s structural solver which solves the full linear elasticity equations. We verified the residual stress implementation by comparison to our coarse-grained solver which solves for membrane displacement using Kirchhoff plate theory, and incorporates the residual stress through a curvature term in the Kirchhoff theory. The problem solved is that of a thin 400 μm membrane of 4 μm thickness. Young’s modulus of nickel is taken to be 200 GPa and Poisson’s ratio is taken to be 0.3. Table 9.2 shows the computed deflection of the metal membrane at two different actuation voltages, 100 V and 160 V, for a tensile residual stresses of 0 MPa and 50 MPa. With a tensile residual stress, the deformation in the beam is less than that without residual stress. It is seen that that results for the structural model using the full elasticity equations match very well with those from the coarse-grained model for these small deflections. For larger actuation voltages close to pull-in, the Kirchhoff theory would tend to deviate from the complete elasticity equations because of the absence of non-linear stretching terms.

### Table 9.2: Comparison of the maximum membrane deflection using MEMOSA-FVM’s linear elasticity model with Kirchhoff plate theory in the presence of residual stress.

<table>
<thead>
<tr>
<th>Applied Voltage</th>
<th>Structure Model</th>
<th>Coarse-Grained Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>100V No Residual Stress</td>
<td>-0.2141 um</td>
<td>-0.214 um</td>
</tr>
<tr>
<td>100V Residual Stress</td>
<td>-0.1183 um</td>
<td>-0.118 um</td>
</tr>
<tr>
<td>160V No Residual Stress</td>
<td>-0.6988 um</td>
<td>-0.681 um</td>
</tr>
<tr>
<td>160V Residual Stress</td>
<td>-0.3337 um</td>
<td>-0.332 um</td>
</tr>
</tbody>
</table>

Fig. 9.8: Comparison of full structural solver and plate element models. (a) creep deformation of membrane center point, and (b) total deformation of membrane center point.

9.3.3 Residual Stress Model

Residual stresses play a critical role in determining membrane deformation in the RF-MEMS switch. Thus far, we have modeled the effects of residual stress in the PRISM device by employing an effective Young’s modulus. During Year 3, we introduced a residual stress term in MEMOSA-FVM’s structural solver which solves the full linear elasticity equations. We verified the residual stress implementation by comparison to our coarse-grained solver which solves for membrane displacement using Kirchhoff plate theory, and incorporates the residual stress through a curvature term in the Kirchhoff theory. The problem solved is that of a thin 400 μm membrane of 4 μm thickness. Young’s modulus of nickel is taken to be 200 GPa and Poisson’s ratio is taken to be 0.3. Table 9.2 shows the computed deflection of the metal membrane at two different actuation voltages, 100 V and 160 V, for a tensile residual stresses of 0 MPa and 50 MPa. With a tensile residual stress, the deformation in the beam is less than that without residual stress. It is seen that that results for the structural model using the full elasticity equations match very well with those from the coarse-grained model for these small deflections. For larger actuation voltages close to pull-in, the Kirchhoff theory would tend to deviate from the complete elasticity equations because of the absence of non-linear stretching terms.

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</tr>
</tbody>
</table>
9.3.4 ES-BGK Implementation

During Year 3, implementation, testing and verification of the ES-BGK model for rarefied gas dynamics was completed in MEMOSA-FVM. In this section we describe the three-dimensional unsteady implementation of Boltzmann-ESBGK solver with the conservative formulation of collision relaxation. In addition, we present results of solver verification that has been carried out by comparison with analytical solutions for a 0D unsteady and a 1D steady flow problem. For 2D gas damping, a code-to-code comparison is performed.

The ES-BGK solver consists of a finite volume method in physical space and a discrete ordinate method in velocity space. The velocity space discretization is implemented using both Cartesian and spherical meshes, as shown in Fig. 9.9. The spherical mesh consists of a 16th order Gauss-Hermite quadrature in velocity magnitude and both the 3/8th rule and constant interval in angle. The velocity is then stored as an array of vectors, where \( c_j = (c_x^j, c_y^j, c_z^j) \), \( j \) is the jth element in the array. From here on, the subscript \( j \) will be dropped when referring to individual components of the \( c_i \) and will be referred to as \( c_x, c_y, c_z \).

The discretization in the physical space is based on arbitrary convex polyhedral meshes. CuBit and Gambit are used to create the meshes for the different tests. The solver has the capability of reading in a Fluent .cas file and the mesh partitioner automatically partitions the mesh. An algebraic multigrid solver (AMG) is used for the solution of these linearized equations. Details for discretization of the convection term, algorithm for implementation of Dirichlet and Neumann conditions can found in Ref. 43.

Five different types of boundary conditions are incorporated into the solver. The first one is a fairly simple one called ‘ZeroGradBC’ which corresponds to no gradient in functional values and macroscopic properties. Two important boundary conditions are the fully-diffuse wall boundary and the symmetry boundary. The solver can also admit a specular-diffuse wall with a given accommodation coefficient and far pressure inlet and outlet boundaries. For each boundary condition, the boundary distribution function is calculated and stored in the ghost-boundary cell. Finally for each linear system in the velocity space, Dirichlet and extrapolation type of boundary conditions are applied for incoming and outgoing directions respectively.

The implementation of the solver in MEMOSA-FVM was completed during Year 3 and extensive testing and verification was undertaken. We present a few verification problems here.

**Time Discretization.** The first verification case was chosen to test the time discretization. A space homogeneous relaxation of a weighted Maxwellian to a single Maxwellian was selected for this purpose. This is a 0D problem that has an analytical solution for the single relaxation-time collision model formulation. The distribution function initialized to a weighted Maxwellian of two flows. The first has a non-dimensional velocity \( u_1 = 1.0 \) and weight \( w_1 = 0.75 \) while the second is described by \( u_2 = 4.0, \ w_2 = 0.25 \). They both have the same density \( \rho \) and temperature \( T \). The initial distribution is

\[
f_0 = 0.25 \frac{\rho}{\sqrt{\pi T_0}} \exp \left( -\frac{(c_x - 4.0)^2 + (c_y)^2 + (c_z)^2}{T_0} \right) + 0.75 \frac{\rho}{\sqrt{\pi T_0}} \exp \left( -\frac{(c_x - 1.0)^2 + (c_y)^2 + (c_z)^2}{T_0} \right)
\]

The steady-state distribution is obtained as

\[
f_M = \frac{\rho}{\sqrt{\pi T_f}} \exp \left( -\frac{(c_x - 1.75)^2 + (c_y)^2 + (c_z)^2}{T_f} \right)
\]
where $T_f = 2.12 \cdot T_0$. The unsteady analytical solution is given by

$$f(t, c) = f_M^t(c) + (f_0(c) - f_M(c)) \exp(-t / \tau).$$

Figure 9.10 shows the iso-surfaces of the distribution function at level $f = 0.001$ using a Cartesian-type velocity meshes of size $14 \times 14 \times 14$ and $26 \times 26 \times 26$ with extent of $c_{\text{max}} = 10.5$. A non-dimensional time step of $\Delta t = \tau/(2RT)^{0.5} = 10^{-3}$ was used for all of these simulations. These solutions obtained for different meshes show good agreement with the exact solution at 3 different instances in time where $t/\tau = 0, 0.85$ and 4.26. Also shown is the solution from a Cartesian-type velocity mesh of size $20 \times 20 \times 20$ with an extent of only 7.5. Notice how the right end of the iso-surface is sliced off at both times $t = 0.0$ and $t = 0.85$. This shows that extent of $c_{\text{max}} = 7.5$ for the velocity domain is not sufficient to capture the entire iso-surface. This difference does not show up in the $L_2$ norm ratio in Fig. 9.10 Therefore, visualization of the distribution function can be useful in determining the correct extent of the velocity mesh for a particular problem. Figure 9.11 shows the variation $L_2$ norm ratio which is a quantitative measure of the deviation from equilibrium solution.

![Iso-surface at level f=0.001 of the distribution function from solver and exact solution at different times.](image)
Entropy can be a powerful parameter in verification of numerical solution to non-equilibrium flows. In this 0-D problem, entropy starts from an initial value of 31.25 and increases with time till equilibrium is reached at 31.85. The different types of velocity discretization converge to different equilibrium states as shown by the final entropy. The final entropy is lower for a coarser velocity grid and increases to reach the exact entropy as the velocity grid is made finer. The $L_2$ norm ratio on the other hand, shows that the convergence to equilibrium is exponential but fails to distinguish between the different final equilibrium states. Entropy generation rate decreases for all velocity meshes to reach equilibrium state with net $dS_{coll}/dt = 0.0$.

**One-Dimensional Couette Flow.** The second verification problem is the one-dimensional plane Couette flow. Specifically this case was used to verify the implementation of the wall boundary condition, in particular, the specular-diffuse Maxwellian model with a prescribed accommodation coefficient $\sigma$. The same case as the one used by Bird\textsuperscript{14} is considered. The gas, argon, lies between two plates $H = 1$ m apart maintained at a temperature of $T_w = T_0 = 273$ K. The bottom wall is at rest while the top is moving with the velocity $u_w = 10$ m/s in the x direction. Initially the gas has a density $\rho = 9.28 \times 10^{-6}$ kg/m$^3$, corresponding to a pressure $P_0 = 0.528$ Pa. For this data, Bird obtains the Knudsen number for his variable hard sphere model as 0.01. For the case $Kn = 0.1$, all conditions are same except the height of the channel is now 0.1 m. A linear profile of velocity is used as the initial condition for all the simulations. Figure 9.12 show the comparison between theoretical and computed velocity profiles for a $10 \times 80$ mesh in physical space and a 10x10x10 Cartesian-type velocity mesh. Three meshes with refinement factor $r = 2$, i.e. meshes with 20, 40 and 80 cells in the y direction are used here. Using RMS error from meshes for the Couette flow problem, the apparent order is found to be $p = 1.8$. It should be noted that the boundary conditions implemented are still only first order accurate.
**Squeeze Film Damping.** The third verification case is a code-to-code comparison for a 2D gas damping problem. Figure 9.13 shows the parallel decomposition of computational domain and boundary conditions. The left, top, bottom, right boundaries are symmetry, pressure-inlet, pressure-inlet and wall boundaries respectively. Mesh and domain size convergence studies were performed for squeeze-film damping of a beam with width $w = 18\mu m$, thickness $t = 2.25\mu m$ and gap-size of $g = 1.4\mu m$. This specific case was picked out to verify the correctness of pressure-inlet and moving wall boundaries. The resulting damping force calculated from the simulation was compared with the 2d compact model\textsuperscript{115} and the error was 5.8% for the 100×100mesh. This error would be further reduced by increasing the velocity grid.

### 9.3.5 Improvements to Parallel Scaling of MEMOSA-FVM

The MEMOSA-FVM solver currently supports four parallel linear solvers: the Algebraic MultiGrid (AMG) solver, the Bi-conjugate Gradient Stabilized Method (BiCGStab) with an AMG pre-conditioner, the BiCGStab method with an ILU pre-conditioner and a BiCGStab with the SPIKE family of pre-conditioners. A domain decomposition method is used to parallelize MEMOSA-FVM.

The focus of Year 3 was to implement SPIKE pre-conditioners in MEMOSA-FVM. The SPIKE pre-conditioner implementation uses Fiedler re-ordering, defined as follows. Let $A$ be a symmetric matrix of order $n$. The weighted Laplacian matrix $L$ for $A$ is given by:

$$L(i,j) = -|A(i,j)|, \quad \text{for } i \neq j$$

$$L(i,i) = \sum |A(i,k)|, \quad \text{for } k = 1,2,\ldots,n; \quad k \neq i$$

We obtain the eigenvector corresponding to the second smallest eigenvalue of $L$:

$$L \times x_2 = \lambda_2 x_2$$

We then sort the Fiedler vector $x_2$ based on the values of its entries to obtain the Fiedler permutation. We
compute the Fiedler vector using the Trace Minimization parallel eigenvalue solver developed at Purdue. We then apply the Fiedler ordering to the rows and columns of A. The reordered matrix has the property that large entries in the matrix are brought close to the main diagonal. After the reordering, we extract a banded approximation to A, and use this pre-conditioner within an iterative method such as BiCGStab, as illustrated in Fig. 9.14. The solution with the banded matrix is done in parallel using SPIKE. The SPIKE solver forms a reduced system based on the coupling blocks (see Fig. 9.15) which is solved in parallel. The remaining solution is computed by a local solve using the diagonal blocks $A_i$. Our implementation uses banded Gaussian elimination as the solver for the $A_i$ blocks. MEMOSA-FVM can also use Metis partitioning initially to partition the domain. The Metis graph partitioner is designed to produce balanced partitions and also minimum communication surface between the partitioned domains. Fiedler reordering does not minimize surface communication between domains but makes the SPIKE preconditioner in MEMOSA-FVM more effective by clustering large elements around the main diagonal.

**Comparison with Hypre.** In Fig. 9.16, we show a comparison of the SPIKE algorithm (using F90 and a hybrid MPI+OpenMP programming model), for a matrix of order 11.3 million unknowns extracted from the pressure correction solution in the MEMOSA-FVM code. This figure compares the strong scaling of SPIKE with that of the parallel algebraic multigrid solver in Hypre, on an Intel Harpertown cluster.

We have also tested the parallel performance of MEMOSA-FVM on the Hera (LLNL) machine. The Hera cluster is a 127 Teraflops/s cluster with 864 nodes. Each node has 4 AMD quad-core Opteron processors (16 cores per node) at 2.3 GHz, and 27.6 TB of memory. The nodes are connected by a fast InfiniBand DDR (Mellanox) interconnect. The 3D lid-driven cavity problem is chosen for the test. The problem consists of laminar Newtonian flow in a cuboidal cavity driven by a moving lid at a Reynolds number of 1.0, as shown in Fig. 9.17. This test case has a mesh with 4 million hexahedral cells. We ran the solver up 100 iterations (momentum relative residual $<10^{-2}$, continuity relative residual $<10^{-4}$) for a mesh of fixed size to perform a strong scalability test.

In Fig. 9.18 we show speed-up and efficiency results for this problem, for four different linear solvers. The SPIKE (semi-bandwidth=5) and ILU0 pre-conditioners give the best scaling results on Hera for MEMOSA-FVM solvers.
A number of infrastructure enhancements were made to MEMOSA-MPM during Year 3. A time implicit algorithm was implemented and tested. The algorithm is a matrix-free implementation of a Newton-Krylov method to solve the nonlinear equations of solid mechanics. We use restarted GMRES for the Krylov space method in order to enable the so-called momentum formulation of MEMOSA-MPM. Even without preconditioning, the implicit solution was demonstrated to be more efficient than the explicit solver on several problems. We found that the deformations are not large for the MEMS switch simulations of this project, so the velocity formulation of the material point method (MPM) can be used. The advantage is that the matrix associated with the discretization is symmetric, positive-definite and the more efficient conjugate gradient method (CG) can be used. MEMOSA-MPM can solve dynamic equations (including inertia terms) either implicitly or explicitly and can solve static equations (equilibrium equations) implicitly using these solvers.

In addition, significant improvements to the parallel implementation of MEMOSA-MPM were made. The parallel version of MEMOSA-MPM is based on domain decomposition. We have demonstrated excellent parallel efficiency on up to 1024 processors for the main time loop. This

---

Fig. 9.18: The speed-up (top) and efficiency (bottom) of lid-driven cavity flow runs on Hera (LLNL) using MVAPICH2.

<table>
<thead>
<tr>
<th>Researchers</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>D. Sulsky, Math, UNM</td>
<td>P. Wallstedt, Math, UNM</td>
</tr>
<tr>
<td>M. Wester, Math, UNM</td>
<td></td>
</tr>
</tbody>
</table>
efficiency holds for both the time explicit and implicit algorithms and also holds for both double and tangent data types, the latter used for linear sensitivity analysis through automatic code differentiation.

We have modified our implementation of MEMOSA-MPM to enhance its parallel performance in various ways. At initiation, the MEMOSA-MPM code executes a preprocessor step that reads input describing the geometry, generates the material points based on that description, and writes a NETCDF file with the material points. The main MPM code reads the NETCDF file and an input file giving other execution parameters, and runs the simulation according to these parameters. The initial implementation passed all I/O through the main node. Using many processors and medium-sized datasets, the overhead for this initialization procedure is large (on the order of an hour for 1024 processors and 4 million cells with 8 particles per cell). We changed the scheme so that each processor writes its own datafile during preprocessing or reads it during execution of the main code. On the same problem, the initialization time using this new procedure dropped down to 2.5 minutes, about a 20-fold improvement, as shown in Fig. 9.19. In the future, we plan to adapt ParaView to read these individual output files from each processor, a capability that this visualization system is advertised to handle.

Performance of GMRES and CG are assessed using an example of a cube being sheared at top and bottom. Figure 9.20(a) shows good weak scaling through 1024 processors, where the problem size is doubled in one dimension when the number of processors is doubled, starting with a single processor problem size of 16 x 16 x 16 cells, 8 particles per cell. For one GMRES / CG timestep set equal to one explicit timestep at CFL conditions, the calculations run 3 (CG) to 4 (GMRES) times slower than the comparable explicit calculation. However, if one GMRES / CG timestep is set equal to 1000 explicit timesteps at CFL, the calculations only run on average 5 (CG) to 7 (GMRES) times slower than the above
explicit calculation, so 200 (CG) to 140 (GMRES) times faster than the comparable number of explicit timesteps. For a single processor problem size of 32 x 32 x 32 cells (close to the maximum possible problem size that can be held in the memory of a single processor), one GMRES / CG timestep set equal to one explicit timestep at CFL, Fig. 9.20(b) shows that both implicit schemes run about 30 times slower than the comparable explicit algorithm. We have not yet run comparable timings for one implicit timestep set equal to 1000 explicit timesteps at CFL.

Another series of calculations examined the effects of the aspect ratio of the sheared cube upon timing results over increasing numbers of processors (see Fig. 9.21). This calculation is relevant to the PRISM membrane which has aspect ratios in the range of 100:1 or 200:1. Starting with a 16 x 16 x 16 cell problem, 8 particles per cell, the length of one dimension of the geometry was doubled (hence, the object is no longer a cube, but can be thought of as a series of cubes stacked up in a column, shearing occurring at the top and bottom). If one processor is used, the timings increase exponentially. However, doubling the numbers of processors as the height of the column is doubled produces nearly constant timings.

9.5 Enhancements to PuReMD
Over the last year, our work on reactive atomistics focused on two major challenges:

- Development of semi-automated methods for force-field optimization.
- Development of new scalable solvers within PuReMD to enhance the scaling envelope of the code.

Beyond these, we continue to support PuReMD and its LAMMPS integration (LAMMPS/ReaxFF-C), through bug fixes, response to feature requests, and supporting analyses routines. We provide a brief description of these developments here.

9.5.1 Force-Field Optimization for ReaxFF
One of the major constraints using reactive force fields is the large parameter space that must be suitably trained, either through experimental or quantum-chemical data, to yield a usable model. The high dimensional parameter space (typically, in the hundreds) and the highly non-linear nature of the objective function make training computationally difficult. The highly optimized nature of PuReMD, coupled with use of large-scale parallel platforms, allows, for the first time, aggressive semi-automated approaches to force-field optimization.

Our implementation of the force field optimization software has been divided into two modules, TrainGen (training set generation), which defines the error function, and FFOpt (force field optimization), which modifies a specified set of parameters in order to minimize the error.
TrainGen generates geometries that sample the configuration space of specified elements. Three-body systems serve to evenly explore bond distance and bond angle energy profiles. For each triplet of atom types, geometries of various bond lengths and angles are generated. These systems primarily explore non-equilibrium configurations. Randomly-generated systems are used to explore equilibrium configurations. For given ratios of element concentrations, atoms are randomly placed in a box. These systems are energy minimized in a multi-step procedure. In each step, the quantum chemical (QC) calculation increases in accuracy and computational cost. Specific systems of interest may also be manually added to the training set geometries.

Observable quantities of the systems are calculated by TrainGen via external QC software (Gaussian). FFOpt input files containing these geometries, associated data, and weights for each data point are generated. The error function is defined by comparing the same data points generated using ReaxFF.

Given this error function, FFOpt seeks to find a point in parameter space of minimum error. As mentioned, optimization is challenging due to characteristics of both the parameter space and the error function defined on that space. The parameter space is of very high dimension, and cannot be considered as orthogonal (i.e., changing one parameter causes changes to others). The error function is not necessarily continuous and may be undefined for certain ranges of parameter values. The domain of the error function may not be known prior to optimization.

A simple method of optimization, already integrated in ReaxFF force field optimization, is to perform a steepest descent type optimization for each parameter individually and iterate over all parameters. This method is sensitive to the order in which parameters are optimized. This can be reduced by taking small steps and running many iterations. A Nelder-Mead type optimization is now being implemented within our framework. This method "tumbles", expands, or contracts a polyhedron defined by N+1 points (where N is the dimension of parameter space) in order to approach a minimum.

---

Fig. 9.22: Improving accuracy of force-field parameters as our optimization procedure executes. Also shown are various other physical quantities that are verified.
At this development stage, both TrainGen and FFOpt are fully functional. TrainGen is an original method developed specifically for this project. FFOpt is an adaptation of an older method. It has been written to allow easy extension to other MD packages, but is currently functional on PuReMD alone. A steepest descent type optimization that performs a parabolic fit when near the minimum is currently implemented. A training set for hydrogen and oxygen has been generated and optimization has been initiated (Fig. 9.22). The choice of this system is motivated by the acknowledged difficulty of generating an acceptable water force field. For a training set, 36,504 three-body systems and 42 random systems were considered. Three-body ground state energies were calculated using the hybrid density functional B2-PLYP with empirical dispersion. Random systems were optimized using (in order): semi-empirical PM6 Hamiltonian, B3LYP with the 6-311G basis set, B3LYP and 6-311G with diffuse and polarization functions, and finally B2-PLYP with dispersion. Atomic point partial charges were calculated by fitting the electrostatic potential using the CHelpG method. Bond order was taken to be the Wiberg bond index in the Natural Atomic Orbital (NAO) basis. Errors were weighted by the number of systems of that type to avoid accumulating too much error from non-equilibrium three-body systems. While this is still work (and indeed, computation) in progress, the percentage of acceptable parameters has increased significantly (Fig. 9.23).

9.5.2 New Scalable Solvers for Charge Equilibration

While PuReMD (and its LAMMPS integration) are easily the fastest reactive MD realizations, currently, there are scaling bottlenecks to the current implementation that become evident beyond a few thousand cores. Figure 9.24 shows the weak-scaling performance of PuReMD on up to 3375 cores. The figure shows that while the performance at this configuration is excellent (overall efficiency over 75%), it also shows that for much larger configurations, this becomes a bottleneck. Specifically, the charge-equilibration solve is a major consideration for continued scaling.

Fig. 9.23: Increase of acceptable parameters in ReaxFF as our optimization procedure has been executing.
To address this, we have, over the past year, initiated development of a new charge-equilibration solver. This solver uses a SPIKE decomposition pre-conditioner (see Section 9.3), in conjunction with a CG solver. SPIKE decomposition has been shown to be significantly better than ILU pre-conditioners for broad classes of linear systems, and is inherently parallel. We have demonstrated parallel implementations of SPIKE that scale to large number of processors. Integrating SPIKE into the Charge Equilibration step, however, requires some additional design considerations. In contrast to many applications, in our implementation of Charge Equilibration, the coefficient matrix is never explicitly constructed. This implies that the SPIKE pre-conditioner must operate on partially constructed kernels. Furthermore, SPIKE is critically dependent on suitable reordering of the matrix. In the case of Charge Equilibration, this is implicitly done through a spatial aggregation of atoms (already implemented in PuReMD for cache performance). With these considerations, we have designed a SPIKE-based solver within PuReMD. This solver is currently being tested for performance, scalability, and error tolerance. We anticipate the next release of PuReMD to incorporate this novel solver, which will significantly enhance the scaling envelope of PuReMD.

Fig. 9.24: Weak scaling results of current PuReMD implementation. Total time per step as a function of increasing number of cores (Hera) and system size is shown. At 3375 cores, the size of the simulated system is approximately 22M atoms. Per-step time for the six major PuReMD components are also shown.
10. EDUCATION AND OUTREACH

A number of important contributions have been made in the education arena in Year 3. These are summarized below.

10.1 PRISM Seminar Series

<table>
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<th>Title</th>
<th>Lecturer</th>
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<tbody>
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<td>1</td>
<td>Intro to V&amp;V and UQ; basic statistics</td>
<td>A. Alexeenko</td>
</tr>
<tr>
<td>2</td>
<td>Linear sensitivity analysis; finite difference, code differentiation</td>
<td>S. Mathur</td>
</tr>
<tr>
<td>3</td>
<td>Uncertainty propagation - sensitivity equation, variance propagation equation, non-deterministic sampling</td>
<td>L. Sun</td>
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<tr>
<td>4</td>
<td>Polynomial chaos - Galerkin and collocation</td>
<td>A. Narayan</td>
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<tr>
<td>5</td>
<td>Polynomial chaos - Galerkin and collocation</td>
<td>A. Narayan</td>
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<tr>
<td>6</td>
<td>Using MEMOSA UQ software</td>
<td>M. Hunt</td>
</tr>
<tr>
<td>7</td>
<td>Uncertainty quantification in experiments</td>
<td>A. Raman</td>
</tr>
<tr>
<td>8</td>
<td>Verification and validation of computational models</td>
<td>A. Alexeenko</td>
</tr>
<tr>
<td>9</td>
<td>Introduction to DAKOTA</td>
<td>B. Pax</td>
</tr>
<tr>
<td>10</td>
<td>Introduction to Bayesian methods and Bayesian calibration</td>
<td>S. Mahadevan</td>
</tr>
<tr>
<td>11</td>
<td>Bayesian networks for uncertainty quantification</td>
<td>S. Mahadevan</td>
</tr>
<tr>
<td>12</td>
<td>Epistemic uncertainty in molecular dynamics; Closure</td>
<td>A. Strachan</td>
</tr>
</tbody>
</table>

Table 10.1: Lecture topics in PRISM seminar course on uncertainty quantification (ME 597/AAE 590).

A seminar series was held in Year 3 to address topics of interest to PRISM research. Speakers in the seminar series represented a broad cross-section of Computational Science and Engineering, MEMS research, and related physics. During Fall 2010, the seminar series was used to offer a 1-credit seminar class (ME 597/AAE590) entitled “Introduction to Uncertainty Quantification.” The class was offered to the entire Purdue community, and was required of all PRISM graduate students. We had 36 graduate students registered, both PRISM and non-PRISM. The lectures were presented by PRISM faculty and staff, and were video-recorded; they are available on http://memshub.org. Lecture topics for the semester are shown in Table 10.1. Seminars presented in the seminar series held in Spring 2011 are shown in Table 10.2.

10.2 Workshops and Short Courses

Members of the PRISM team attended the PSAAP workshop on V&V and UQ held in Austin, Texas, in July 2010. PRISM researchers also organized a 2-session symposium on uncertainty quantification at the 2010 ASME IMECE held in Vancouver, BC, in November 2010. Profs. Aluru and Murthy were invited speakers at the NNIN/C Symposium in MEMS/NEMS Simulation held at University of Michigan, Ann Arbor, during April 2011.
10.3 Course Contributions to CSE Curriculum
During Fall 2010 and Spring 2011, a number of graduate level courses were offered by PRISM faculty under Purdue’s Computational Science and Engineering program. These are listed in Table 10.3. In addition, a seminar course, “Introduction to Uncertainty Quantification,” (ME 597/AAE590) was also taught, as described above.

<table>
<thead>
<tr>
<th>Date</th>
<th>Speaker</th>
<th>Affiliation</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>2/11/2011</td>
<td>Mr. Shankhadeep Das</td>
<td>Purdue ME</td>
<td>“A Finite Volume Method for Stress Analysis with Application to MEMS”</td>
</tr>
<tr>
<td>2/18/2011</td>
<td>Prof. Ananth Grama</td>
<td>Purdue CS</td>
<td>“Emerging Opportunities, Challenges, and Applications in Exascale Computing”</td>
</tr>
<tr>
<td>4/1/2011</td>
<td>Prof. W. Crossley</td>
<td>Purdue AAE</td>
<td>“Some Examples of Design under Uncertainty for Aerospace Problems”</td>
</tr>
<tr>
<td>4/8/2011</td>
<td>Dr. Allison Hartzell</td>
<td>Lilliputian Systems</td>
<td>“MEMS Reliability”</td>
</tr>
<tr>
<td>4/28/2011</td>
<td>Prof. Vikas Tomar</td>
<td>Purdue AAE</td>
<td>“Experiments and Models Regarding Strain Dependent Thermal Conductivity and Strength at the Nanoscale and Microscale”</td>
</tr>
</tbody>
</table>

Table 10.2: PRISM seminar series for Spring 2011.

10.4 Summer Internships
During Summer 2010, four students went to the Labs as interns. During summer 2011, two students went to the Labs for internships. Details are given in Table 10.4. One post-doctoral fellow (Hojin Kim) is tentatively scheduled to go to LANL in Summer/Fall 2011. This brings the total number of PRISM graduate students who have interned at the Labs to 12. Furthermore, two PRISM students have found employment at the Labs: Abby Hunter (LANL) and Robert Sayer (Sandia). Hasan Metin Aktulga, another PRISM graduate student, has found employment at Lawrence Berkeley Labs.

<table>
<thead>
<tr>
<th>Course Number</th>
<th>Instructor</th>
<th>Course Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>CS 525</td>
<td>A. Grama, Purdue</td>
<td>“Parallel Computing”</td>
</tr>
<tr>
<td>CS 505</td>
<td>A. Grama, Purdue</td>
<td>“Distributed Computing”</td>
</tr>
<tr>
<td>AAE 590</td>
<td>A. Alexeenko</td>
<td>“Molecular Gas Dynamics”</td>
</tr>
<tr>
<td>MA 692D</td>
<td>S. Dong, Purdue</td>
<td>“High Performance Computing”</td>
</tr>
<tr>
<td>ME 608</td>
<td>J. Murthy</td>
<td>“Numerical Methods for Heat, Mass and Momentum Transfer”</td>
</tr>
<tr>
<td>CS 51500</td>
<td>A. Sameh</td>
<td>“Numerical Linear Algebra”</td>
</tr>
<tr>
<td>CS 51501</td>
<td>A. Sameh</td>
<td>“Special Topics – Parallelism in Numerical Linear Algebra”</td>
</tr>
</tbody>
</table>

Table 10.3: CSE courses taught by PRISM faculty in Year 3
10.5 Summer Undergraduate Research Fellowships

During the summer of 2010, two undergraduates are being supported under Purdue’s Summer Undergraduate Research Fellowship (SURF) program.

10.6 MEMShub Development

Development of MEMShub, a web-portal for MEMS-related research continues. MEMShub leverages the HUBzero software platform for scientific collaboration (http://hubzero.org) developed by Purdue’s Network for Computational Nanotechnology (NCN). The software framework developed during Year 1 was extended, and web resources continue to be added. Improvements to the Purdue Coarse-Grained solver (PCGS), which allows the simulation of approximate models of the PRISM device, continue to be made. Furthermore, we have made available videos and Power-point slides of the PRISM seminar course on uncertainty quantification on this website.

Table 10.4: PRISM students in internships at the National Laboratories during 2010-2011. (*) Tentatively scheduled for Summer/Fall 2011.

<table>
<thead>
<tr>
<th>Student</th>
<th>Laboratory</th>
<th>Lab Advisor</th>
<th>PRISM</th>
</tr>
</thead>
<tbody>
<tr>
<td>N. Anderson</td>
<td>Sandia</td>
<td>P. Schultz</td>
<td>A. Strachan</td>
</tr>
<tr>
<td>A. Hunter</td>
<td>LANL</td>
<td>T. German</td>
<td>I. Beyerlein</td>
</tr>
<tr>
<td>B. Pax</td>
<td>Sandia</td>
<td>K. Dowding</td>
<td>J. Murthy</td>
</tr>
<tr>
<td>P. Madrid</td>
<td>LANL</td>
<td>R. Lebensohn</td>
<td>D. Sulskey</td>
</tr>
</tbody>
</table>

Fig. 10.1: A view of MEMShub (http://memshub.org)
11. PERSONNEL STATUS
A list of PRISM personnel in Year 3 is shown in Table 11.1.

<table>
<thead>
<tr>
<th>Name</th>
<th>Role</th>
<th>Citizenship</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jayathi Murthy</td>
<td>Center Director</td>
<td>USA</td>
</tr>
<tr>
<td>Matt Potrawski</td>
<td>Managing Director</td>
<td>USA</td>
</tr>
<tr>
<td>Stephanie Bonebrake</td>
<td>Center Secretary</td>
<td>USA</td>
</tr>
<tr>
<td>Ahmed Sameh</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Alejandro Strachan</td>
<td>Faculty</td>
<td>Argentina</td>
</tr>
<tr>
<td>Alina Alexeenko</td>
<td>Faculty</td>
<td>Russia</td>
</tr>
<tr>
<td>Ananth Grama</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Anil Bajaj</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Arvind Raman</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Ashraf Alam</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Deborah Sulsky</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Dimitri Peroulis</td>
<td>Faculty</td>
<td>Greece</td>
</tr>
<tr>
<td>Dongbin Xiu</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Mariisol Koslowski</td>
<td>Faculty</td>
<td>Argentina</td>
</tr>
<tr>
<td>Narayan Aluru</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Sanjay Mathur</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Suchuan Dong</td>
<td>Faculty</td>
<td>PRC</td>
</tr>
<tr>
<td>Tim Fisher</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Wayne Chen</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Sankaran Mahadevan</td>
<td>Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Aravind Alawan</td>
<td>Grad Student</td>
<td>India</td>
</tr>
<tr>
<td>Abigail Hunter</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Andrew Kovacs</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Ankit Jain</td>
<td>Grad Student</td>
<td>India</td>
</tr>
<tr>
<td>Josh Mullins</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Aarti Chigullapalli</td>
<td>Grad Student</td>
<td>India</td>
</tr>
<tr>
<td>Shankhadeep Das</td>
<td>Grad Student</td>
<td>India</td>
</tr>
<tr>
<td>Bob Sayer</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Hao Han Hsu</td>
<td>Grad Student</td>
<td>Taiwan</td>
</tr>
<tr>
<td>Hasan Metin Aktulga</td>
<td>Grad Student</td>
<td>Turkey</td>
</tr>
<tr>
<td>James Loy</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Jeremy Nabeth</td>
<td>Grad Student</td>
<td>France</td>
</tr>
<tr>
<td>Jia Li</td>
<td>Grad Student</td>
<td>PRC</td>
</tr>
<tr>
<td>Joshua Small</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Kyoungmin Min</td>
<td>Grad Student</td>
<td>PRC</td>
</tr>
<tr>
<td>Michael Snow</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Murat Manguoglu</td>
<td>Grad Student</td>
<td>Turkey</td>
</tr>
<tr>
<td>Nathan Anderson</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Patrick Cantwell</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Pedro Madrid</td>
<td>Grad Student</td>
<td>Honduras</td>
</tr>
<tr>
<td>Ryan Tung</td>
<td>Grad Student</td>
<td>USA</td>
</tr>
<tr>
<td>Sambit Palit</td>
<td>Grad Student</td>
<td>India</td>
</tr>
<tr>
<td>Sruti Chigullapalli</td>
<td>Grad Student</td>
<td>India</td>
</tr>
<tr>
<td>Vedula Ravi Pramod</td>
<td>Grad Student</td>
<td>India</td>
</tr>
<tr>
<td>Kumar</td>
<td>Grad Student</td>
<td>India</td>
</tr>
<tr>
<td>Yingchong Situ</td>
<td>Grad Student</td>
<td>PRC</td>
</tr>
<tr>
<td>Ben Pax</td>
<td>Graduate Student</td>
<td>USA</td>
</tr>
<tr>
<td>Gabriela Venturini</td>
<td>Post Doc</td>
<td>Argentina</td>
</tr>
<tr>
<td>Hojin Kim</td>
<td>Post Doc</td>
<td>S. Korea</td>
</tr>
<tr>
<td>Phil Wallstedt</td>
<td>Post Doc</td>
<td>USA</td>
</tr>
<tr>
<td>Akil Narayan</td>
<td>Post Doc/Visiting Faculty</td>
<td>USA</td>
</tr>
<tr>
<td>Mike McLennan</td>
<td>Research Staff</td>
<td>USA</td>
</tr>
<tr>
<td>Gazi Yildirim</td>
<td>Research Staff</td>
<td>Turkey</td>
</tr>
<tr>
<td>Lin Sun</td>
<td>Research Professor</td>
<td>PRC</td>
</tr>
<tr>
<td>Faisal Saied</td>
<td>Research Professor</td>
<td>USA</td>
</tr>
<tr>
<td>Martin Hunt</td>
<td>Research Staff</td>
<td>USA</td>
</tr>
<tr>
<td>Michael Wester</td>
<td>Contractor</td>
<td>USA</td>
</tr>
</tbody>
</table>

Table 11.1: List of PRISM personnel
12. CENTER PUBLICATIONS


A. Hunter, I. Beyerlein, T. Germann and M. Koslowski, "Incorporation of partial dislocation in a phase field dislocation model", Materials Science and Technology Conference and Exposition, Houston, TX, October 2010.


H. Kim and A. Strachan, “Molecular dynamics study of the contact strengths between clean metallic surfaces with nanoscale asperities”, American Physical Society March Meeting, Dallas, Texas, March 2011.


M. Koslowski, "Design of materials with improved mechanical properties", XXXI Iberian Latin American congress on Computational Methods in Engineering (MECOM2010), Buenos Aires, Argentina, November 15


13. REFERENCES

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