



# Center Response to Recommendations from October 2010

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*R1: We encourage you to continue to refine and evolve the coarse grain model so it can be used as a testbed for making predictions*

- a. Use the coarse grain model in the end-to-end system for an early understanding of multi-scale and multi-physics interdependencies*
- b. Consider applying the Bayes network approach to the coarse grain model and capture the lessons learned*
- c. Incorporate a coarse grain model for creep and contact.*
- d. Refine behavioral physics of residual stress in the model.*

These recommendations have already been acted upon.

- We have incorporated a creep model in both the coarse-grained model and MEMOSA.
- A contact model based on Prof. Strachan's work has been incorporated in both the coarse grained solver and in MEMOSA.
- A residual stress model has already been incorporated in both.
- We have used the coarse-grained model as a testbed to work out all the Bayes network pathways. We have used the lessons learned in full-system simulations with MEMOSA. You saw some of it this morning and you will see more this afternoon.

*R2: Define phase for implementing Bayes' network into MEMOSA. Any improvements to lower the computational cost of gPC uncertainty propagation would be welcomed.*

- We have developed a step by step plan for incorporating Bayes networks in MEMOSA, as you have seen in Talk 1.
- Regarding lowering gPC cost, we are employing a number of approaches such as sensitivity analysis and tier-wise elimination of unimportant variables. We first do sensitivity analysis using our coarse-grained model, and limit the number of random variables in our MEMOSA simulations.

*R3: In order to make progress on the stated predictive goals in years 4 and 5, dielectric charging, contact and creep need to be integrated in an end-to-end numerical simulation, at least to some extent, in the coming year 3.*

- We have already taken the first shot at this work
- We have computed creep+electrostatics in MEMOSA-FVM for 800 hours on the frogleg device. We have used this information to calibrate the creep model and have predicted PRISM device creep+electrostatics.
- We have performed UQ of PRISM device pull-in and pull-out. These integrate deformation, electro-statics and contact.
- We have performed UQ of PRISM device sustained contact dielectric charging, pull-in and pull-out.
- We have performed preliminary simulations of multi-cycle PRISM device sustained contact dielectric charging, pull-in and pull-out.

*R4: Consider adding other validation tests for model aspects such as creep that will not be tested by validating the model's ability to predict failure under accelerated testing.*

*Continue to build a culture within PRISM where uniform nomenclature of UQ is used*

- We have used creep data for the frog-leg device to calibrate our creep model. These are not accelerated testing data.
- We are collecting new creep data on the cantilever device, and we will use some of that for validation. These are not accelerated testing data either.
- We hope you saw a jump in the UQ awareness of our faculty, staff and students this year. We will continue to push the culture of PRISM in this direction.

*R5: The UQ study of 1-2 months cycle time in the center plan is somewhat concerning. We suggest a more refined estimation of number of runs and time they will take to plan for several UQ iterations in years 4 and 5.*

- The creep and sustained contact simulation goals are not a concern. We have completed several of these. Each run is about 8 hours on 8-16 processors depending on mesh size and time duration. We are doing hundreds of these runs and have not had difficulty with this. Using the coarse-grained model to eliminate unimportant variable has been very successful. Using surrogate models within the Bayesian framework has also made the Bayesian analysis quite tractable.
- The multiple cycle contact simulation is the biggest issue. Current estimates are that we can run ~10 cycles in a week. The primary bottleneck is not numerics or scaling – it is that the current damping model is very strongly damping near contact. Thus, getting the membrane to pull out takes a lot of time, covered by small time steps which are not parallelizable. We are in the process of running large displacement damping simulations using ES-BGK to see if the near-contact damping behavior can be made more realistic.

*R6: Consider carefully the model form of the Bayesian network approach.*

Prof. Mahadevan and our modeling groups are thinking about this. As you will see, there are critical (and open) research questions this afternoon.

*R7: Define the taxonomy of the (uncertain) parameters such that their fundamental impact on the model is well understood; this will pay dividends in assessing physical correctness of the resulting model and in computational time by decoupling parameters when appropriate.*

This is good advice and it is what we are trying to do in our hierarchical approach to system simulation. We will take it into account as the Bayesian network and UQ work advance.

*R8: Carefully consider the computational cost of handling uncertainties, particularly using sparse grids that have a reliance on simulation convergence at every point.*

This is indeed a concern, not only from a computational cost view point, but also due to the extreme requirements for robustness and convergence it places on our solvers – getting things to work at  $\pm 5\sigma$  on operating parameters is no joke. This is an open research topic at this point, however.

*R9: Refine CPU estimates of calibration and UQ processing times in order to identify possible practical computational issues when using the Bayes analysis*

It is certainly true that Bayesian analysis can engender high cost if the full models are used. The use of surrogate models built using our gPC approach has made this tractable, as we will demonstrate this afternoon.

*R10: Consider the effectiveness of using a bounding model-form approach to fluid damping UQ if the adaptive switch from Navier-Stokes to ES-BGK cannot be worked out over the next year*

We may be forced to do this if the coupling between the two regimes does not work robustly. Also, even with ES-BGK, we will need to approximate near-contact damping. We are working on this open research issue.

*R11: Continue toward incorporation of creep and plasticity models and large deformation squeeze film damping simulations and other coupling strategies between the fluid-structure and electrostatics*

- We have completed the implementation of creep and plasticity in both full structural solver and in our plate element model. The formulation is general and admits other plasticity models readily.
- We have been computing large deformations in the presence of fluid damping through Year 3, and it is a part of our Year 4 end-to-end simulations. Prof. Alexeenko's group is currently working on this.

*R12: We support the continued development of the ES-BGK model within the FVM framework for rarefied gas dynamics near contact.*

This is an open research problem. Prof. Alexeenko has begun to address this in Year 3, and it will continue into Year 4. There are many opportunities using MEMOSA to explore this near-contact behavior, especially in the presence of roughness – there would be significant contributions to the science. But the resources we will expend on this will depend on how much difference it will really make to the ultimate goal of lifetime prediction.

*R13: If ReaxFF becomes too expensive to achieve the PRISM goals, consider intelligent ways to develop approaches that link ReaxFF methods to considerably less computationally expensive interatomic descriptions (such as EAM or MEAM).*

This is an open research topic, but an interesting one. We will think about this.

*R14: Continue to refine the connection from lower (atomistic) levels to mesoscale models.*

*In particular, we suggest further analysis of the suitability of the atomistic creep simulation period being currently investigated (e.g. 1-2 cycles) and of the connection between high strain rates in simulation vs. low strain rates in experiment*

We are sorting out the connection between atomistic and mesoscale levels for creep, tentatively through the yield stress term in the creep model. At present our simulations and experiments are for the same conditions – we are not running high strain rates in our simulations and low ones in our experiments. The creep simulations are not being done under accelerated testing conditions.

*R15: Explore adopting formal design of experiment methods in order to minimize the total number of simulations required for uncertainty propagation (i.e., tap into the existing expertise in the center in this area)*

We have thought about this in the past, but opted to go for sparse-grid based gPC instead. We may revisit this if the cost of gPC becomes too onerous.

*R16: Strongly consider comparing simulated pdfs or first few moments to experimental results for evaluating the reliability of the system under the three scenarios that describe the PRISM prediction goals.*

We are working with Prof. Mahadevan to get beyond the mean-to-mean comparison as a validation metric. His Bayesian validation work does allow us to consider statistical information in making validation decisions using the Bayes factor idea. You will see some results from this approach this afternoon.

*R17: Interaction with experts in design of experiments on the team is going to prove particularly useful in paring down the raw number of measurements necessary to achieve statistical significance in experimental validation tests.*

This is a good suggestion and we will work with Prof. Mahadevan on this.

*R18: To put process variation into perspective, we recommend an evolving quantitative estimation of the models' predictive dependence on process and device information. For example, this estimation would reveal whether process flow information alone is adequate to predict a device's performance or if more detailed information required (i.e., run information, tool information, test structures on a specific device, etc.). For devices, such estimation would guide knowledge of what amount of characterization detail is necessary to adequately predict the average device performance.*

The idea of removing device geometry related uncertainty from the estimation of overall uncertainty to understand the epistemic contribution is a good one, and we have done some of this in Year 3. For example, in predicting pull-in voltage, we first addressed a specific device (#2-3D) and predicted its behavior without getting into pdfs of geometry etc. But we do feel that if device variability is the main determinant of prediction uncertainty, that should come out of the simulation exercise.

We are not entirely certain what you mean by process flow information. It would not be easy in our view to include computationally the details of the fabrication process, tooling etc.

*R19: Consider measuring thickness, gap and stress on all experimental devices and selecting those that are substantially the same so you emphasize the effects of the other parameters. For example, perhaps this could be done by picking devices over a small area of a given wafer.*

Yes, we are already doing this. We always try to do deterministic simulations first on well-characterized devices to get a handle on how well the basic models are working. We then work in variability in geometry, properties etc.

*R20: We suggest that you experimentally quantify residual stress, using test structures, given its stated importance.*

We are working on this. One way being explored by Prof. Arvind Raman, is to correlate device modal response to residual stress. Some modes of vibration of the device, for example the torsional modes, appear (theoretically) to be independent of residual stress, while others depend on it. Therefore, it may be possible to use this idea to measure Young's modulus independent of the residual stress. This would give us a way of estimating residual stress independently.

Alternatively we are using cantilevers in which differential stress, resulting in membrane curvature, is possible to characterize more easily. This allows us to calibrate properties and model constants without getting tangled in a hard-to-measure quantity like residual stress.

*R21: We suggest you perform post and pre mortem work on experimental devices and correlate to your failure data.*

We will look into this and see if useful pre- and post-mortem analysis can be done.

*R22: Emphasize achieving an approximately equal number of internship appointments at all NNSA laboratories when appropriate.*

It is our desire to do this, but a lot depends on the overlap between lab and PRISM activities. This year we have sent students to LLNL, in addition to Sandia. Hojin Kim will spend Nov 2011 at LANL. Please be assured that it is on our radar.

*R23: Continue to refine planning in order to create more internships of longer duration (12+ weeks)*

We are trying to find students at a suitable point in their careers that can afford to do this. It is not easy.

*R24: Continue looking to enhance cross-disciplinary engagement across the entire PRISM community, like the successful UQ seminar series and the MEMSHUB*

We are trying to do this, and will continue.

*R25: Incorporate the Executive Advisory Board meeting findings and recommendations into next year's review process.*

We will do this (see end of this presentation).

*R26: Reach out to other PSAAP Centers to share successes and lessons learned, particularly with respect to software development.*

We organized a symposium at IMECE 2011 in which all PSAAP centers made presentations on their work. We have participated in symposia organized by the PECOS center in Feb 2011 and this summer. We also participated in the PSAAP UQ workshops, held this year at Stanford. We had Bob Moser visit and give a PRISM seminar 2 weeks ago. In addition, we have some collaborative activity to individual members of the other centers. We will stay open to these exchanges.

*R27: Continue to refine flow of information and to refine your research plan for out years.*

We are doing this.

*R28: Consider turning your red/yellow/green (stoplight) chart into a true Gantt chart.*

We can do that, but have not found them to be particularly helpful in the past.

*R29: Refine your metrics for the three goals in Year 5 to reflect better the mission of predicting reliability.*

We will continue to do this.

*R30: We are sensitive to your resource limitations, but we urge you to think about simulating at least one different design per condition in order to show prediction capability in Year 5.*

Integrating data and predictions from different devices has emerged this year as a central feature of our calibration and validation efforts. You will see more on this in the afternoon today.

*R31: Create one or more tables or charts showing the switch design parameter space (with values used in experimental designs and priorities for testing vs. year), as these will be helpful tools to understand the path for validation and assessing predictive capability.*

We have these laid out for the devices being used for the current simulations and will have them for future devices as well. The operation space is well-defined at this point.

# TST Review Feedback

## June 2011

# DAY 1 TST DISCUSSION

- Clarify progress in context of full-system UQ
- Will a full Bayesian network have been exercised by October?

We are confident that the creep Gen 5 Bayesian network (Goal III) will be exercised by October. (We have done this with the frog-leg already).

There is also a reasonable probability that we can take a crack at the Goal II Bayesian network (pull-out under sustained contact). We may not have the experimental data that we need yet, but uncertainty propagation can be demonstrated and the Bayesian methodology laid out for the most part.

Goal I using MEMOSA will probably take longer if sufficient cycles are to be done efficiently, primarily because of the near-wall-damping issue. But the general approach can be played out using the coarse-grained model by October.

- Will Bayesian approach be used to inform decisions regarding coupling FVM model to 1) MPM and 2) ES-BGK models? If not, what approach will be used?

There is no “coupling” to be done. The fluid, structure, electrostatics, ES-BGK, creep and contact all sit in MEMOSA-FVM. We just turn on the requisite models on during a run. So we are not sure what you are asking...

We have not yet completed hooking up ES-BGK to IBM to allow us to do fluid-structure interaction with ES-BGK (i.e have the structure move through an ES-BGK fluid rather than a Navier-Stokes fluid). The preliminary algorithms have been worked out outside MEMOSA, and implementation is underway.

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- What coupled physics are fully operational in MEMOSA? In particular, what are the options and trade-offs being considered for simulating a beam moving through a fluid background?

Please see above – we have all we need in MEMOSA-FVM at this point except ES-BGK integration with IBM (need to put in boundary conditions). We expect this to be done in the next 2 months. We also have not yet done adaptive switching between ESBGK and NSSJ but can probably do our simulations without this for the moment.

We have 2 types of structural models in MEMOSA-FVM at this point: (i) a full-fledged solution of the 2D or 3D linear elasticity equations, and (ii) a plate element model based on Mindlin-Reissner theory. Both are fully-integrated with the NSSJ solver and electrostatics through IBM.

In terms of tradeoffs between the full elastic structural solver vs the Mindlin-Reissner plate element model – we find that for  $L/h > 100$ , the plate element model does very well. If we don't encounter thick membranes, the plate element model will probably be our workhorse. It certainly has been these last 3 months.

In terms of tradeoffs in the fluid model – if we can get the near-wall contact issue sorted out, we may be do mainly NSSJ, with some ES-BGK to bound error (the cost issue is key for unsteady ES-BGK).

## What would you have to do to have first UQ simulations for all three goals by October?

For Goals II and III, we have largely completed the first shot at simulations, response-surface building and a preliminary Bayes network setup and computation. Refinements are needed as well as incorporation of new cantilever data as they emerge. But the pathway is now clear.

For Goal I, we have taken a preliminary shot at multicycle simulations but have not yet done a serious integration with Bayes networks.

Emphasize UQ to drive your efforts.

Yes, we're trying to do that.

Has Maha assumed UQ technology leadership?

Yes, it is his vision that is driving the entire Bayes network, calibration and validation ideas.

How are Maha's UQ approaches spread to Purdue et al.?

Maha has given 2 lectures on his Bayesian approach in our UQ seminar class (see memsHUB). PRISM researchers are beginning direct collaborations with him on other projects.

We talk every Friday during our weekly UQ Steering Group meeting.

He and his students have access to PRISM codes and wiki, and have computer accounts at Purdue. So far our interactions have involved having his students run PRISM coarse-grained models and of Purdue students providing him the necessary gPC response surfaces from MEMOSA to be used in the Bayes network. We also provide experimental data and error bars.

This summer, we had a group of Purdue students spend time at Vanderbilt . They worked with Maha and his students to understand Maha's Matlab codes for calibration. We now have a number of students who are using these methods and codes at Purdue.

Mike, Martin, Jayathi and Sanjay also visited Vanderbilt in September to understand how the Bayes network idea could be integrated into our UQ environment MEMOSA-UQ. Preliminary work on this has begun.

Maha visited us in October and worked with a number of PRISM researchers to pull their models and experiments into to the Bayesian framework.

## Continue progress in verification

Will the verification studies be rigorously documented?

Yes, we have a system for checking in verification and validation tests into our version control and regression testing system. We write up a description of each test in our test matrix and check in the corresponding script to run MEMOSA.

- **What are your 5 big “aha”s from last year?**
  - Resolved multiscale connections in dielectric charging
    - Role of multiple trap depths (pdfs) in explaining charge vs time - entirely new
  - Resolved multiscale connections in contact modeling
    - Role of roughness, uncertainty in material properties, hardness in pull-out prediction
      - entirely new
  - Bayesian network analysis of creep
    - Ability to pin-point model form uncertainties from analysis
  - Completion of main models, numerics and software
    - Contact computation, efficient plate element model, ES-BGK
  - Predictive computation of pull-in in Gen 5 with UQ,
    - Good match with measurements

# EAB Feedback from March 2011

# Questions for EAB

Question 1: Are we adequately fulfilling the “Predictive Science” mission of the PSAAP program ? As you know, the primary focus of the PSAAP program is on uncertainty quantification. Have we made good progress?

Question 2: What should we be doing to engage the MEMS community? One of our goals is to make our work visible to the MEMS community and to become more aware of their issues.

Question 3: Do the research/codes/methods developed in the Center have legs? What possible future directions can we take?

Question 4: The NNSA has announced that Phase II of the PSAAP program will involve exascale computing and will involve an open competition. Do you have any thoughts on the opportunities in this area and what we could be doing to pursue them?

# Response #1

Question 1: Are we adequately fulfilling the “Predictive Science” mission of the PSAAP program ? As you know, the primary focus of the PSAAP program is on uncertainty quantification. Have we made good progress?

- Need to put the models together and make predictions including quantifying uncertainty within the next year
- Why aren't current models being applied to available data? We suggest utilizing available external empirical models and data as well.
- Need to put the models together and make predictions including quantifying uncertainty within the next year.
- Is the end goal clearly stated? How is success defined?
  - Is prediction of failure still a component of the program or is the primary focus the prediction of the materials?
  - What data do you plan to utilize to complete the predictions?

# Response #2

Question 2: What should we be doing to engage the MEMS community? One of our goals is to make our work visible to the MEMS community and to become more aware of their issues.

- Progress is acceptable with the efforts made to date.

# Response #3

Question 3: Do the research/codes/methods developed in the Center have legs? What possible future directions can we take?

- Other opportunities have been suggested in the summary slide.

# Response #4

Question 4: The NNSA has announced that Phase II of the PSAAP program will involve exascale computing and will involve an open competition. Do you have any thoughts on the opportunities in this area and what we could be doing to pursue them?

- UIUC can play an important role in this effort
- Opportunities for exascale computing
  - Dielectric charging
  - Atomistic level modeling – temperature dependence of friction, diffusion, creep, low-cycle and high-cycle fatigue, spallation, corrosion, etc.
  - Mesoscale device modeling
  - Aging component integrity and assessment
  - Consider more complex system of multiple devices

# Additional Recommendations

- Time is of the essence – this next year is important to merging milestones and consolidating individual program components
- Continuity of presentations from previous year to this year – need to clearly indentify incremental progress

# Summary

- From the EAB's point of view, the program has made progress towards meeting many of last year's recommendations.
- Other items still remain as pertinent recommendations such as:
  - High level program plan that includes specific milestone and contingencies
  - Merging the individual models - more clarification is needed
  - Probability of risk and impact to be recorded
  - Industry focus in phase II
  - Suggested future expansion
    - FVM code and others with gradients are attractive to industry – start a Masters or PhD thesis focused on this code for industrial use – maybe partner with a software vendor (ex. Ansys??)
    - Mesoscopic simulation of fatigue
    - Molecular dynamic simulation of friction, diffusion, and spallation
    - General mathematical framework to deal with statistics of small sample sizes
- Student posters and presentations were very well done