Role of Computational Mechanics in Industry

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During the final day of the USNCCM conference 2021, a panel session on the Role of Computational Mechanics in Industry was moderated by Dr. Timothy Truster, an associate professor at the University of Tennessee, and Dr. Varun Gupta, a Computational Scientist at the ExxonMobil Upstream Research Company. This panel of invited speakers was organized by the moderators and the conference technical committee to discuss current mechanics trends in industries and laboratories as well as fostering fruitful collaborations and the transition of computational methods from academia to industry. The backgrounds of the five panelists are as follows:

1. Dr. Robert Ferencz leads Lawrence Livermore National Laboratory's Computational Engineering Division which is a group with over 200 technical staff across a range of computational science and engineering fields. He and his group support a variety of programs across the energy and defense sectors both in labs and industry. Before joining LLNL, Bob was among the founders of a multiphysics simulation software firm in the private sector.
2. Dr. Vinay Goyal is a Principal Engineer at Aerospace Corporation in the Los Angeles area where he has more than 20 years' experience in the aerospace industry. He is responsible for ensuring the technical integrity of risk assessments for several aerostructures, and one of his particular areas is for space launch vehicle reuse certification. He currently serves on to NASA NESC technical teams and has co-authored half a dozen standards. Both Vinay and Jacob were planning a similar industry-academia intermixing symposium at an AIAA conference that was cut short due to COVID and were happy to contribute at USNCCM this year.
3. Dr. Jacob Rome also works with Aerospace Corporation as a Senior Project Leader in the Structures Department. He has spent 2 decades evaluating composites and other complex parts for National Security Space programs, including nozzles, liquid rocket engines, and other components. Prior to joining Aerospace Corp, Jacob earned his MS and PhD in Mechanical Engineering from UC San Diego.
4. Dr. James Sobotka is a senior research engineer at Southwest Research Institute in San Antonio Texas. His research and development in computational mechanics is targeted at support of structural integrity decisions. A few examples include additive manufacturing process modeling, verification and validation of novel constitutive models, and development of new stress-intensity factor solutions for engineering fracture mechanics software. James is an alumnus from the University of Illinois at Urbana-Champaign with his PhD in Structural Engineering in 2010.
5. Dr. Xiao-Hui Wu is a Senior Principal Computational Scientist at ExxonMobil with their Upstream Integrated Solutions Company. He has led multiple R&D projects with teams from academia, laboratories, and industries on topics such as reservoir modeling, multiscale methods, and inverse problems. His current focus is on integrating data sciences and physics-based models to support decisions under uncertainty. Xiao-Hui joined ExxonMobil in 1997 after his postdoc in Applied Mathematics at Caltech and his PhD from the University of Tennessee in Mechanical Engineering.

A lively discussion followed between the panelists and the prepared questions interspersed with audience questions and comments. An abridged interview/transcript from the panel and the chat is given first, followed by a summary of key themes and recommendations for USACM.

First question from Dr. Varun Gupta: What is the role of Computational Mechanics at your company/organization? And would you say yours is a typical example for your industry/field?

The responses from each panelist are summarized as follows:

Dr. Sobotka: The research at Southwest Research Institute (SwRI) is funded by the contracts between the Institute and the clients in the industry. SwRI writes proposals for industry problems and, upon selection, SwRI provides credible solutions to problems generally on the applied technology space. Computational mechanics is a tool for that process. In general, current methods are suitable for problems in industry. New methods may need to be developed In the rare case where current methods are not good enough.

Dr. Wu: Computational mechanics really underlies many of the important decisions we make in the oil and gas industry from exploration and development of oil and gas fields to improving refinery efficiencies and producing better consumer products. In upstream oil and gas sector, when we talk about physics-based models, we primarily mean computational mechanics models. One of the commonly used tools we apply is reservoir simulation which solves complex multiphase flow problems in porous media. Actually, reservoir was invented in ExxonMobil in 1950s to 60s and we have a long history in developing various computational mechanics technologies.

Dr. Goyal: In Aerospace Corporation, we use computational mechanics a lot. One of their primary customers is NASA, and the computational mechanics is applied heat transfer, cohesive elements, applications on hypersonic delamination, and a variety of other problems.

Dr. Rome: In Aerospace Corporation, continuum mechanics is pervasive, lots of physics-based modeling like NASGRO software, putting more emphasis on additive manufacturing. We know what machines do and we can measure it. A key thrust now is, how do we connect that with simulation, data monitoring and integrating huge datasets with high fidelity modeling?

Dr. Ferencz: Computational mechanics and simulations are the foundation of their laboratory, dealing with unique problems that cannot be captured in consensus standards and design practices. They analyze and certify complex assemblies and structures, utilize exotic materials, highly energized, complex environments, multiphysics, and maintain scientific function over the decades. Working in a national lab, you don't know what you will work on lifetime, nuclear reactor modeling, geophysics and seismic response, additive manufacturing, etc.

The second question asked by Dr. Garikipati, professor at University of Michigan, was about data science and data driven methods. In computational mechanics there are two sides of the coin: data driven modeling versus using data science on its own. Can you speak about these two roles of data driven modeling and how does it apply to your context and where do you see that going?

Dr. Sobotka: SwRI treats data science as a different animal from computational mechanics; they complement each other and work in tandem. Physics-based modeling provides input that data science needs to calibrate models. We tend to keep the data science aspects outside of the physics-based modeling. There have been some efforts recently to push the data science inside the physics-based modeling. It could be fruitful if it is possible to use insights from data science to improve the physics-based modeling. However, it would be better to extract these insights from the data science approaches and embed them inside physics-based models. This approach will generally provide more efficiency, is more satisfying in general, and we are not comfortable using black boxes. Ultimately, we are on the hook to explain to the client what is going on. We can't do that with a black box.

Dr. Wu: In oil and gas research, the approach depends on the stage in which your asset is in. In the development stage, there are huge uncertainties and there is not much data available. For example, in a 10km by 10 km area, we may only have one or two well penetrations sampling the subsurface formation.

We also use seismic data but the resolution is not at the scale we need to predict the fluid flow. We link these data to the decision process through the physics-based model. As you gain more remote sensing data over the asset life cycle, like repeated seismic imaging, you form a better understanding of the field, but still for important decisions we rely on physics-based modeling and computational mechanics. Our main challenge is how to combine the variety of data and physics together.

Dr. Ferencz: Wrapping data science around simulation and experimentation simultaneously, they try to look at both of these extremes of big data and use the data science to collectively steer that enterprise. Asking questions like: What is the next simulation that would add the most value? Or what is the physical experiment that will best help you retire an uncertainty? More broadly there are some terminologies like cognitive computing ascribed to these themes and right now because of the complexity of our software stack, embedding the data science techniques down at the foundation of that is a longer development for us.

Dr. Goyal: They use data science in so many areas in aerospace, trying to understand the data, understanding a process or find specific features in the data that otherwise could not be seen. Also, they use it to understand the sensitivity of variables in different problems and doing Monte Carlo simulations to understand the impact and uncertainty.

Question three asked from the audience was about atomistic or molecular modeling. All of the panelists mentioned that they work only in continuum modeling area.

Question four was asked by Dr. Arif Masud, the organizer of USNCCM conference: We have lately observed about the low participation of industry in the USNCCM conference. Probably part of the reason is that the advanced computational mechanics formulations often get stuck in academia. So can you provide a fruitful example of a cooperation between industry, lab and academia, and what would you say the best practice that might translate to other situations?

Dr. Ferencz: In many industrial organizations, commercial software is the gatekeeper to what is made available to people. In national labs we develop our own software stacks. Here is a nice story that encompasses the basic algorithmic research that happened in my lab, Dr. Mike Puso, in collaboration with Dr. Tod Laursen and one of his students from Duke University. This collaboration let us to move from one of our the traditional areas of contact algorithm, posed the challenge and we got to leverage Mortar contact to get into embedded mesh methods, and used that as a vehicle to attack multiphysics problems, by co-executing multiple codes and bringing their strength. Multiple years of internally funded project hosted the student for summer internship, and eventually she did postdoc there. Also, we had incubation of basic methodology development. We are quite fortunate to have 5 or 6 year of contract funding through HPC modernization of DoD, really productized that methodology and made it highly parallel implemented. This is a spin out of academic research and productize technology that is available in a NL.

A follow up question was asked by Dr. Masud on how to increase the participation of industry in this conference.

Dr. Rome: It just ties with how it can be applied as illustrated by an example from a collaboration with UCLA for several years on high fidelity simulation of nondestructive evaluation technics. Basically, from scratch, it was simulation of propagation, very intensive and correlative with actual data. We bridged the data with simulation through artificial intelligence techniques. We interact with contractors as we know that if the research is successful, it will have clear application in industry. That’s what get people interested, if they can see the path from successful research to an application. Sometimes the research is very interesting, but the question is what one would do with that. Is that something we can practically use? When the research is motivated by an objective that get into practice, that's what gets the industry interested and make them come to events like this if they know these tools can be applied.

The follow up question from Dr. Masud was the outcome of USNCCM is the collaboration between researchers and helps promote the research and product of this entire enterprise is the high-quality students and researchers as a community produced, and industry hires all of that. So, what can we do to have the industry come and participate?

Dr. Wu: At least in ExxonMobil we encourage computational scientists to participate in conferences, except the last two years because of the pandemic. We do have lots of participation as it is a good recruiting venue for the company. The challenge is, there is some detachment between research and industrial applications. One of the key indicators of any uptake in industry for new research or technology being developed in academia is the level of interest and energy research shows in helping industry, to address challenging practical cases. Most times in academia, some prototype technology is developed to demonstrate that it works and it is an interesting idea, but that is 20% of actual work to get it to the finish line in order to have a robust and reliable practical application. We have to spend a lot of time on edge cases that are on the edge of assumptions you have. That is where the challenge is, and we have to work them out and they are not necessarily good publication materials. Collaboration between research institutions and industry, sustained collaboration would help the process.

The follow up question from Dr. Masud was about sustained collaboration. There is an addition to cutting edge research, from industrial point of view, there are a lot of loose research that need tightened before industry gets involved in it, but how can we still bring the industry in the process that it will be done, as industry could be a larger part of the USACM portfolio.

Dr. Sobotka: There is a real need for there to be an application for the research. One example of fruitful research between academia and industry has been the AM process modeling. It is not perfect, but a lot better than couple years ago. It has been integrated into high end modeling simulation tool like Abaqus, and involved everybody from industry, the labs, and academia. Critically, it involved solving a practical problem of real quantities, that could be measured. The experimental work provided the credibility to the computational work. It ensured that the focus of the work was not lost. It also kept everyone honest.

Another question from Dr. Masud was that if you were to organize a symposium and bring industry to the USACM, what would you do differently to attract more people from industry.

Dr. Goyal: The US congress in computational mechanics is very specific and does great job with high quality works. There is a potential fear that it does not a lot of industry participation. Industry participation in other conferences is basically by reaching out to the community looking at potential applications. For example, we have had several publications in computational mechanics topics, and we would potentially submit a paper at this conference and highlight our collaboration. Reaching out really aggressively does a great job as people in the industry are busy having the work done and looking for more practical conferences to attend. But bringing that to my light is fruitful for me, and some excitement from what is going on here. In addition to that, it is reaching out, engaging with our community. Most of the papers are highly theoretical and at the end, didn't tell you how to connect it to the real life. If we can teach students how to give a very good motivation and explain the bigger picture perspective and the objective of the research by saying how you can use it 10 years from now.

The last question was asked by Dr. Yuri Bavilevs. The question is as follows. We have quite many PhD students and Postdocs. Some of them are inspired to continue their career in academia, but a lot of them are inspired to go to a national lab or industry. What are some of the tips for success you would give to students, and what do you expect from them? Specifically, if you can define what success means in your lab, what knowledge or skill you need in your organization?

Dr. Ferencz: In federal national labs we exist to go after complex problems. People who want to be successful have to be open to collaboration, be patient, invest time and learn other disciplines terminology. Young staff have difficulty with the sense of knowing when to ask for help. Most of us have been strong students and put any problem to the ground. When we enter professional organizations, spending two weeks on something that if you asked someone else, they could help you in twenty minutes. It doesn't mean they are smarter than you, they have more experience and contact. Ultimately, we should decide what success looks like. There is great uncertainty on everyone's career, know that you have to make decision with imperfect knowledge, make your best decision through yourself with passion. Even if you do not end up what you expected, you will have the richest experience along the way.

Dr. Wu: One advice to students and postdocs, in companies try to fall in love with problems, not the solution. In academia, we tend to stick to a certain idea and push that. In industry often you need to change that based on the problem you face. People who are successful tend to be curious and open minded, focus on what matters, and continuously learn throughout their career.

Dr. Sobotka: Dr. Sobotka: We need people who are flexible, can communicate, and work well with others. If you want to be flexible, you have to have skills beyond what you learned in your thesis. Learning a scripting language (Python, R, Julia), and tools like Mathematica, Git, etc. is important. The most fundamental tools are (for better or worse) Word, Excel, PowerPoint, and Outlook. Keep open mind on solving a problem, expect to find some inertia in doing things in certain ways.

Dr. Goyal: Be passionate about what you do, go to internships, and learn that life can change quickly, so try to be adaptive.

Summary of key responses from panelists:

- Physics-based modeling and a variety of computational mechanics tools are used extensively across the disciplines represented by the panel.
- Data science techniques have been used to quantify uncertainty, for surrogate models, and in various other ways to complement physics-based models. Some disciplines/industries are using physics-based models and data-driven approaches in an integrated fashion while others are more distinct and targeted at different stages of overall problems.
- Often, advanced computational mechanics formulations get stuck in academia. One barrier is that in many industrial organizations, commercial software is the gatekeeper to what is commonly used. An alternative is the closed or open source software stacks being developed at the national laboratories, particularly the latter. One example cooperation between industry, Lawrence Livermore National Laboratory, and academia was on the transition of the lab's contact mechanics software to tackle embedded and moving interface problems and ultimately be scaled up to a highly parallelized environment that is available in software products. This project was supported by the DoD HPC modernization program and lasted several years starting with internships of a couple students from university coming to the lab and later one becoming a postdoc, in close tandem with the faculty members. Another example from SwRI on three-way collaboration is the problem of additive manufacturing linear process modeling. This platform developed over several years with integration of high-end modeling simulation tools like Abaqus and experimental measurements with breadth and

depth to provide credibility to the modeling. The radically different simulation approach resulted in a paradigm shift that needed a large-scale education effort in industry to accept the approaches.

- Another reason that cutting edge research gets stuck in academia is that there are loose end cases beyond the core proof of concept, and these cases may not be suitable material for publication due either to intellectual property issues from industry side or the perception of increment work from the academic side. In other words, some prototype technology can demonstrate a workable and interesting idea, but that is 20% of the actual work to get it to the finish line in order to have a robust and reliable practical application. Sustained collaboration between research institutions and industry can overcome these pitfalls. From the industry side, being able to see and envision a clear application in industry is very important. That path from successful research to applications 10 years from now is a big driver of interest and motivation. Training students and presenters at conferences like USNCCM to provide this longer-term perspective within their talks can go a long way to attracting more industry participants to come to this conference.
- In addition to hearing concise research motivations and vision for long term tools for application, the conference already has substantial energy for theoretical, sound, and cutting-edge work. These two are assets that need to be actively communicated to industry through some engagement and outreach. By considering some key thrust areas of the conference and targeting industries in those sectors, a broader awareness can be achieved in these industries. To begin, start with some key areas of potential application and aggressively reach out to industries, who otherwise may be busy getting done and are in the habit of attending more practical conferences. Bringing to light the longer-term payoffs of sustained collaboration can provide the value proposition to increase participation from industry.
- Tips for success for graduate students and postdocs going into industry and laboratories:
    - People who want to be successful have to be open to collaboration, be patient, invest time and learn other disciplines terminology.
    - Foster a sense of knowing when to ask for help, being humbler and inquisitive to learn from others with more/different experience.
    - During the uncertainty of one's career path, you will have to make decision with imperfect knowledge, so carry through your decision with passion and create a rich experience along the way.
    - Try to fall in love with problems, not the solution. People who are successful tend to be curious and open minded and focus on what matters and continuously learn throughout their career.
    - Industry and laboratories need people who are flexible, can communicate and collaborate.
    - Be passionate about what you do, go to internships, and learn that life can change quickly, so try to be adaptive.