Integrated Computational Materials Engineering

Digitally Improving Products by Integrating Materials, Process Engineering and Manufacturing

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IN BRIEF

Like coffee, steel today has many types: you can get your own mix, and quick. At the time of this writing there are 3500 grades of steel,[1] and at every reading of this there will be many more. Though steel is still produced like a commodity, this is fast changing and is getting closer to the end product needs. Your car needs to be lighter; your canned food needs safer packaging; your home needs prefab steel that can lock into place; the steel type (or "product") for each is changing with demand for improved performance. A similar demand for customization is happening to other materials.

Exciting new computational capabilities are allowing materials engineers to look at Integrated Computational Materials Engineering (ICME) approaches to meet end product requirement with quality, speed and reduced cost. TCS' process engineering lab with its experience in modeling and simulation based solutions for the materials and manufacturing industry and the software engineering lab with expertise in model driven software engineering, have come together to create a futuristic platform for ICME. This platform is for knowledge assisted, simulation driven and data supported engineering. In creating it, the team has addressed some foundational problems relating to the manufacturing industry.

Every material – steel, aluminum, magnesium or exciting new composites such as carbon nanotubes reinforced polymers, functionally graded materials - need to be rendered in an ever changing cocktail, closer to user needs. Because of the pressures of the need for precision, speed and cost savings, there is a sure and firm thrust in the direction of Integrated Computational Materials Engineering (ICME). This *in silico* methodology holds high promise for business, with benefits such as speed (cuts product development time, in some cases, by 15-25%[1]);

1 http://d3em.tamu.edu/wp-content/uploads/2016/04/Report-TMS_icme_study_2013PDF.pdf

Fact File

TCS Research: Integrated Computational Materials Engineering (ICME)

Outcome: TCS-ICME Platform

Principal Investigators: B P Gautham and Sreedhar Reddy

Academic Partners: India (IIT Kanpur, Bombay and Madras), USA (Purdue, Georgia Tech and Oklahoma) and Germany (Aachen).

Techniques used: Manufacturing modeling, design engineering, machine learning and knowledge engineering; model driven Software Engineering

Industries benefited: Manufacturing, Energy and Resources, Hi-Tech, Life Sciences, Engineering & Industrial Services.

Patents: 10 filed

Papers: 15 journal papers, 30 papers in conference proceedings and 4 book chapters.

quality (gets the quality required with fewer iterations; reduces wastage. Lowers the chance of the material failing the product requirement); and reduced cost (Ford's Virtual Aluminum Casting (VAC) project recorded an RoI of 7:1 with a saving of millions.[2]).

We present here the motivation for moving towards ICME, the technology enablers, the strengths of TCS' ICME platform, and the future as we see it.

Challenges in materials engineering

In the manufacture of materials, the success of a product depends on many things: understanding the nature of the raw materials under different conditions; finding the right blend; the right processing conditions to achieve desired properties; the process engineering that is required for scaling up production; and the actual manufacturing efficacy.

While the manufacturing process has benefited from automation and digitization, materials and process engineering are just beginning to take baby steps towards leveraging digital technologies. Some issues that persist include:

Silos: Deep silos exist between different engineering departments. The materials engineering and product design departments know less about the variability and economies of manufacturing. Manufacturing department has limited knowledge of the microstructure of material and its impact during production and the final outcome.

Knowledge gaps: In the old fashioned way of improving processes and creating better products, organizations had generations of learning; there were a limited number of products, and engineers spent their careers in a single industry and even a plant. Today, there is a surge in

2 http://www.tms.org/portal/PUBLICATIONS/Studies/ICME_Implementation_Study/portal/Publications/Studies/ICME_Implementation_Study.aspx?hkey=21689c88-89b2-46da-a2e8-1929dfd2a205

new products, new technologies and attrition in the workforce. That means there is not enough knowledge on the new areas; and we cannot always depend on the tacit knowledge of people.

Data abundance: However, there is an abundance of data about the physical and chemical nature of materials as well as enormous data collected from the manufacturing processes and products in service with the penetration of IoT. Product development as well as manufacturing systems can benefit from leveraging this.

Complexity: Product engineering is getting ambitious - from pharma to auto, industries are looking at combining more and more distinct materials. The raw materials, the combinations, the process sequences and the parameters for each can be varied so much, that it needs an integrated and computerized approach to assist experimentation.

Emerging technology enablers that impact materials engineering

Advances in modeling and simulation, the ability to leverage large amounts of data from various sources, enormous computing power and capabilities, and digital representation of information and knowledge open up new possibilities for materials engineering.

- The physical behavior of materials can be modelled across a length scale range: from nano particles at atomistic scale to structures at meter scale. Understanding the structure and properties of material at each level is growing at a rapid pace; predictions of mathematical modeling and simulation of their performance under different conditions is growing closer to real world experimentation results.
- With enormous amount of data available, we can use state of the art machine learning to bridge the gaps and augment physics driven simulation
- It is technically possible now to integrate various operations related to materials, product engineering, process engineering, manufacturing and field performance on a single platform, offering a valuable line of sight across the entire product life cycle.
- It is possible to make informed decisions and carry out optimization across the value chain to enhance a number of KPIs (key performance indicators)
- Every iteration towards creating the material, process or product with the required information can be stored as a 'digital thread'. This information adds to the digital documentation of the materials and products. This machine readable data in a standardized language (ontology) about any material, its structure, properties, physical and chemical changes under treatment becomes a book of knowledge. The same applies to manufacturing processes and products.
- This data can further be processed and mined to create additional knowledge for future use

Combining modelling, simulation, AI and knowledge engineering requires a platform approach. Our experience at building platforms using model driven engineering techniques are the key technological aspects driving the TCS ICME Research Program.

TCS ICME Platform

TCS ICME Platform is a software platform that is defined as a 'knowledge assisted, simulation driven, data aided integrated engineering of products – design, manufacturing and materials.'

If TCS' ICME Platform's capability can be represented in layers, we would describe it as follows (see Figure 1):

Layer 1: As part of its core, it provides for a formal representation of materials-manufacturing-products-design. We have used our model-driven-engineering capability for this framework and a number of metamodels representing products, processes, materials, simulation tools, knowledge etc. in an integrated framework. These metamodels are used for representation of data as well as knowledge related to the system.

Layer 2: The next layer involves knowledge-assisted construction of engineering decision workflows based on the designer's intent and the context at hand.

Layer 3: Within the workflow, a number of entities such as simulation tools, external data, micro-services, etc. can be constructed and/or reused. Knowledge elements represented in various forms using the ontology can be contextually provided to the user with applicability rankings or invoked automatically based on the need and case.

Layer 4: Finally, a learning layer is used to mine for patterns and infer relationships from the past

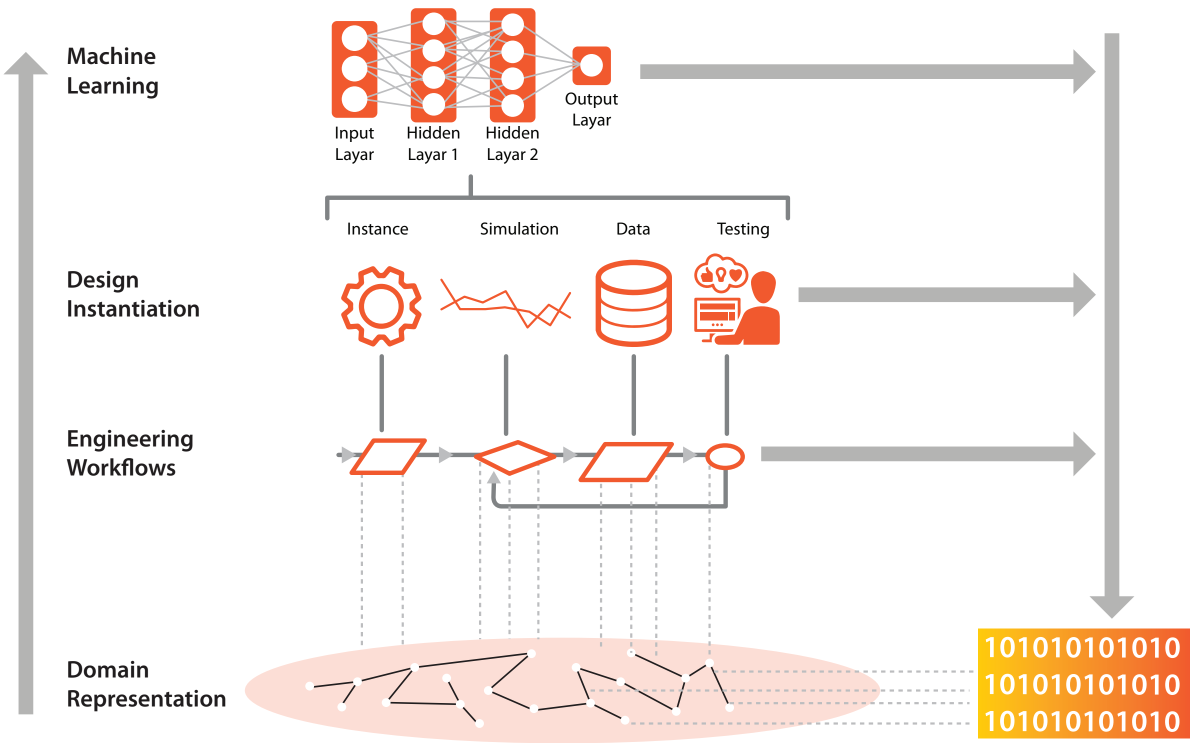

Figure 1: *The architecture of TCS' ICME Platform*

executions and decisions to enhance the knowledge repository as the user keeps creating and improving the product, material, and process designs. Within this, we have also developed complex domain-specific search engines to extract knowledge from documents and we are further working on developing systems for automated curation of this knowledge.

While developing all these concepts, we have worked on three key foundational problems relevant to the manufacturing industry – the first dealing with product and manufacturing process integration, the second dealing with process-scale up, and the third dealing with complex multiscale material design. We have used these as technology demonstrators with relevant engineering research as vehicles for establishing the basic features and utility of our platform.

Unique aspects of TCS' ICME Platform

Designing and deploying materials in products in the most efficient way requires a reasonable view of manufacturing and product design aspects to the materials engineers and similar applies to product design engineers to know materials structure and processing to design optimal products. The TCS process engineering lab in Pune has scientists and engineers who have worked for nearly three decades in modeling and simulation of materials and manufacturing processes and helped customers on all aspects of materials, manufacturing and design with deep materials insight provided through modeling and simulation. The TCS software lab in Pune has experts in model driven software engineering, modeling knowledge, and developing knowledge engineering systems. Both teams came together to create TCS' ICME platform and its extension to product engineering from the perspective of knowledge assisted, simulation driven engineering. This unique collaboration set with a vision as stated in Figure 2 has resulted in bridging the value chain across research to innovation to a platform. Architected on model-driven engineering principles, besides providing a strong semantic basis for expression of knowledge and information, it automates generation of implementation artefacts such as database

Develop tools, technologies, and a digital platform for enabling integrated design of materials, manufacturing processes and products, using a combination of physics based simulations, data driven reasoning and guided experiments, supported by decision support tools and knowledge engineering systems.

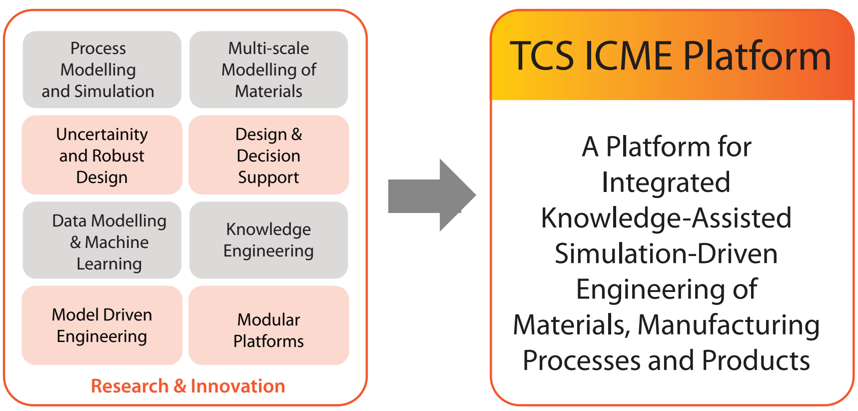

Figure 2: *TCS ICME Platform*

Our vision is to position the TCS ICME Platform as a cloud-based collaborative platform for product engineering for original equipment manufacturers (OEMs), materials suppliers and tier 1 manufacturers with strong domain capabilities.

schemas, workflows, user-screens, and tool adaptors. This provides flexibility to the platform, making it easily customizable for a variety of applications. Leveraging the domain expertise in the lab, TCS ICME platform offers a number of ontology and knowledge engineering features related to materials, manufacturing processes, product systems, simulation tools, etc. giving it an edge over other platforms used for ICME and product engineering.

Research collaborations

During this journey, we have collaborated with many reputed academic and research institutions across the globe and people in different fields. Our key collaborations spanned multiple institutions in India (IIT Kanpur, Bombay and Madras), USA (Purdue, Georgia Tech and Oklahoma) and Germany (RWTH Aachen). Some of these collaborations are TCS funded, some of these are through our colleagues pursuing PhD, and some through multi-lateral initiatives.

We have also created significant IP with more than 10 patents filed till date and many more in the pipeline. We also made a significant impact on the ICME research community through papers and publications with over 15 journal papers, 30 papers in conference proceedings and four book chapters.

We are recognized as one of the few major research groups in the world in ICME, and more so in the industrial research pertaining to ICME. We have participated as a member in ICMEg – the European consortium for standards for materials. We also had representation in the organizing committee of the flagship World Congress on ICME organized biennially by TMS USA ICME2018.

As a leader in the area of ICME in India, we have been prime organizers of many multi-lateral workshops and effectively made the Indian academia and government recognize ICME.

Working with customers

All along, we have been in touch with our business teams, and through them with our customers, to validate and fine-tune what we are doing. We are undertaking initial pilots with our customers through our manufacturing, Energy and Resources, Hi-Tech, and Life Sciences units, and with the EIS and IoT horizontals.

A framework developed by our business team for advising on the feasibility and selection of the right process for additive manufacturing (or 3D printing) is jointly implemented on the TCS ICME platform, and hosted on TCS Cloud. We are also deploying this in academia starting with Indian Institute of Technology, Kanpur and Indian Institute of Science, Bangalore.

The future

Some engineers still scoff at modelling and simulation. But this is the way forward. As pioneers in the field of ICME, we will look at advancing knowledge in this area. We will continue to further expand ontologies, knowledge engineering, simulation and modelling features. We will contribute to standards and to the maturity of this field. Formal capture of this and other forms of relevant knowledge digitally to help carry out all these activities is the icing on the cake.

Our vision is to position the TCS ICME Platform as a cloud-based collaborative platform for product engineering for original equipment

Integrated Design of Gears

Designing a gear that meets user specified functional and performance requirements is a challenging task. The designer has to deal with conflicting goals, such as high reliability, low costs, and compactness. High reliability demands gears of larger size and high-strength material, which conflicts with the compactness and low cost requirements. The cost-to-size ratio is also not linear as smaller size gears can be made using expensive heat treatment and other manufacturing processes. There are a number of possible routes to manufacture a gear, such as:

(a) Blanking → Gear Hobbing → Carburization-Quenching → Tempering → Fine Grinding

(b) Hot Forging → Form Grinding → Carburization-Quenching → Tempering → Fine Grinding → Shot Peening.

In this case study, we limited the study to the design chain involving American Gear Manufacturer's Association (AGMA) based gear design, material selection, carburization-quenching and tempering processes (here in referred to as the CQT) process) and their impact on the gear performance. Figure 3 shows a schematic describing the scope of the current study. It illustrates key steps of a typical process route to be followed while carrying out industrial gear design and manufacture.

We use a standard design code based on AGMA specifications for preliminary design of the gears obtaining a robust design using compromise Decision Support tool (cDSP). The heat treatment models account for thermal analysis, diffusion of carbon during carburizing phase, phase transformations and residual stress evolution at quenching stage and empirical corrections for tempering processes. Material properties are predicted using a combination of mixture rules and empirical correlations based on phase distribution. Finally, the fatigue analysis is carried out taking into account the spatial distribution of the

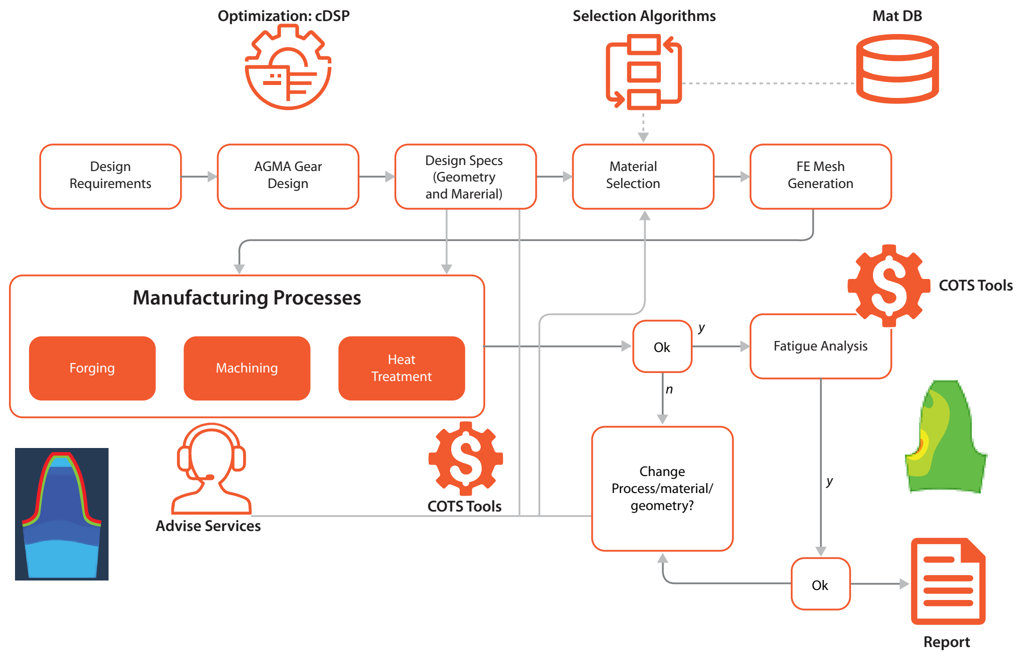

Figure 3: *Process for gear design and manufacture*

material properties as well as residual stresses. The heat treatment simulation tools are built on commercial Finite Element software tools with appropriate user defined functions to take into account the specific metallurgical aspects. This entire workflow is implemented on the TCS ICME platform in such a way that a designer not having any expertise in simulation, can effectively use this for making design decisions.

The design process starts with capturing functional requirements and progresses through geometric design, material selection, prediction of effect of manufacturing process parameters on the properties of the gear component, and finally the evaluation of fatigue performance under design loads. A workflow for integrated design of gears including a sequence of processes along with the knowledge guided assistance is implemented on the TCS ICME platform. Knowledge assistance is provided at several places in the workflow to facilitate decisions on process parameters, to fetch appropriate data from the database and to perform informed corrective actions to achieve the specified targets. Integration of various steps of the design process is accomplished through seamless data interchange using appropriate process and product templates.

Finally, through this integrated route, we have shown that it is possible to obtain a right set of parameters for heat treatment conditions, coupled with design and performance analysis that can lead to 25% reduction in the weight of the gear. We are working with an industrial partner to validate our findings.

manufacturers (OEMs), materials suppliers and tier 1 manufacturers with strong domain capabilities. In the long-term, the platform could also become a first-of-its-kind knowledge and simulation driven processes in adjacencies.

BP Gautham

Gautham is a Principal Scientist at TCS Research and Innovation and leads the ICME research group. He is involved in design automation and in bringing manufacturing process simulation to product design. His other interests are Process Modeling, Simulation and Optimization of materials processing (metals, polymers, ceramics). He has expertise in advanced FEA and solid mechanics. He has worked extensively with various industries solving process related problems through a combination of experiments and simulation tools. Gautham has published about 50 papers in journals and conferences in the areas of process modeling and simulation, design and decision support, FEA, structural dynamics and materials processing. He has a PhD in Structural Dynamics from IIT- Madras, India.

Sreedhar S. Reddy

Sreedhar Reddy is a chief scientist at TCS Research and Innovation. A key member in a team of early pioneers of model driven engineering that developed TCS MasterCraft, a product for enterprise application generation, Sreedhar played an active role in the standardization efforts of the Object Management Group (OMG). He was one of the principal authors of OMG standards 'MOF Query/View/Transformation specification' and 'MOF Models to Text transformation specification'. He has a masters degree in computer engineering from IIT Kharagpur. He has served on the program committees of ISEC, APSEC, MODELS and ICSE. With close to 30 years of experience in areas such as language processing, model driven engineering, modeling tools, databases and knowledge engineering, he has around 40 publications and 7 granted patents.

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