MECH5601: CREATIVE PROBLEMS SOLVING COURSE SYLLABUS

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Contents

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1. Syllabus Mech5601

The creative problem that this course tries to solve is creating an optimal design of a mechanical structure in the early stages of a design. The role of computer algorithms, software systems, software frameworks in modern mechanical engineering is explored. The emphasis is on more holistic computer models that combine experimental data (big data and statistics) with science based theories, e.g., continuum mechanics, reversible and irreversible thermodynamics that are beginning to be integrated into the design process in industry. The emphasis is not on the details of how to use CAD, NC machining, computer control or finite element analysis software packages that are currently used routinely and intensively in industry. The emphasis is on the next steps of how these tools can be integrated into the process of optimizing the design of new products.

To get a sense of what is possible in designing new products today, watch the YouTube video by Space-X on what is arguably the current state of the art in computer models for design.

https://www.youtube.com/watch?v=txk-VO1hzBY

Most software packages that are used to optimize the design of mechanical structures satisfy the conservation laws of energy, mass and momentum as constraint equations. These constraints are most simply expressed in terms of continuum mechanics. The finite element method is the most popular method to solve such problems. Space-X is essentially using only one solver pattern to solve all the problems described in their video.

This is my second year in teaching this course on-line and my first year in using Brightspace. Because of Covid-19, professional organizations and conferences are switching to virtual meetings using TEAMS and ZOOM. Online teaching and conferencing is an opportunity to learn an exciting new capability and to avoid spending time in airports and money on aeroplane tickets and hotel rooms.

In 2021 the final grade in this course will be based on 50% of a Final exam and 50% on exams during the term.

2. Some questions to think about that are relevant to this course.

- Your first assignment is to Google the quotation: **All models are wrong.** What does this quotation imply and why is it important?
- How do you know what to believe and what to trust? In Wikipedia, explore Occams razor, Verification, Validation and Uncertainty Quantification Causality.
  See Stanford Encyclopedia of Philosophy : Rationalism vs. Empiricism https://plato.stanford.edu/entries/rationalism-empiricism/
- What limits the capability of industry to make more use of computer models?
- What is the basis of design of modern aeroplanes, nuclear reactors, ships, etc.?
- Verification and Validation of computer models: The tension between science-based models and experiment-based models. Google a Guide for Verification and Validation in Computational Solid Mechanics Transmitted by L.E. Schwer, Chair PTC

60 /V&V 10. This document provides guidelines that a decision maker should consider when deciding if a computer model for computational solid mechanics should or should not be used to provide information to make a particular design decision.

- Statistics, big data, analytics and deep learning. Computer models range from pure science to pure experimental models. Watch the Hollywood movie Money Ball to see how computer models have changed baseball and most sports. These computer models are based on statistics, i.e., observations of data for real games.
- You are encouraged to Google and watch some of videos of keynote talks by Jen-Hsun Huang, CEO Nvidia and Nvidia videos on manufacturing at some of the Nvidia GPU conferences.
- Google The Way We Think, Vannevar Bush, Atlantic Monthly, July 1, 1945. http://www.theatlantic.com/magazine/archive/1945/07/as-we-may-think/303881/

  This is a remarkable example of one remarkable person predicting the future with remarkable accuracy in 1945. Others may prefer the books written by Jules Verne.

3. Weekly Topics

3.1. **Week 1 Sept 4, 2021 Computational Weld Mechanics.** Arc welding is a complex manufacturing process in which an electric arc generates heat in an area approximately one cm^2 while travelling at speeds of approximately 1 to 5 mm/s to form a pool of liquid metal with volume usually slightly less the 1 cm^3. As the liquid metal on the trailing edge of the weld pool solidifies, a weld joint or weld overlay is created. The transient temperature field from the weld pool drives metallurgical phase changes, thermal expansion-contraction and changes temperature dependent properties of the materials. The microstructure evolves as it is heated and cooled with phase changes, annealing, recrystallization and grain growth. The strain due to thermal expansion-contraction, phase changes and restraint of the structure and fixtures generates stress and plastic deformation. The plastic deformation leads to residual stress and deformation. The mechanical properties of the microstructure in the Heat-Affected Zone (HAZ) largely controls the in-service performance of the welded structure.

The goal of this lecture on computational weld mechanics is not to make you an expert welding engineers. It is to show you that the algorithms to compute 3D transient temperature, microstructure, stress, strain and displacement do not depend on welding. The same theory and algorithms that are used in modelling welds and welded structures can and should be used in all mechanical engineering design problems. They are similar to the algorithm using in the software used by Space-X. All structural design problems become problems in computational continuum mechanics.

3.2. **The conservation of energy in a small cube.** Given a small cube with edge length a, face area a^2, volume a^3. The thermal conductivity is κ. The specific heat is c_p. The spcific enthalpy is h. A flux $q = -\kappa \Delta T/a$ is applied to each face of the cube. The initial temperature is T_0.

Rate at which energy is applied to the cube is face area of the cube $6a^2$ times the flux q.

The rate at which the specific enthalpy h of the cube changes is

$$\frac{dh}{dt} = c_p \frac{dT}{dt} \tag{1}$$

The enthalpy in the cube is $a^3 h$. If all of the flux of heat that flows into the cube in one second heats the cube, i.e., energy is conserved, then the conservation of energy equation is

$$a^3 \frac{dh}{dt} = a^3 c_p \frac{dT}{dt} = 6a^2 q \tag{2}$$

We have assumed that the flux is small enough that the gradient in temperature in the cube can be ignored, i.e., the variation of temperature in the cube in space can be neglected. We have also assumed that no changes in phase occurs and that c_p and κ do no change with temperature.

Next let's divide this equation by a^3.

$$\frac{dh}{dt} = c_p \frac{dT}{dt} = 6\frac{a^2}{a^3}q \tag{3}$$

Next, let's look at the term $6\frac{a^2}{a^3}q$ more closely. In particular, suppose the length of the cube goes toward zero? Then in this limit, the term $6\frac{a^2}{a^3}q$ is called the divergence of the flux and denoted $\nabla \cdot q = -\nabla \cdot \kappa \nabla T$. This is the Laplacian operator.

Let's rewrite the conservation of energy equation with the divergence of the flux.

$$\frac{dh}{dt} = c_p \frac{dT}{dt} = \nabla \cdot q \tag{4}$$

Let's rearrange the conservation of energy equation

$$\frac{dh}{dt} - \nabla \cdot q = 0 \tag{5}$$

Next, let's suppose that instead of applying a thermal flux to the boundary area of the cube, some power density heat source source such as microwaves are heating the little cube at a rate of $Q\ watts/m^3$. Since energy is conserved, the conservation of energy equation becomes.

$$\frac{dh}{dt} - Q = 0 \tag{6}$$

Suppose both the power density Q and the thermal flux are applied simultaneously to the little cube. We can add the two equations because the right hand side is zero to generalize the conservation of energy equation for our little cube.

$$\frac{dh}{dt} - \nabla \cdot q - Q = 0 \tag{7}$$

We can replace $dh = c_p dt$ and $q = -\kappa\frac{\Delta T}{\Delta x}$ and replace $\frac{\Delta T}{\Delta x}$ by the partial derivative $\frac{\partial T}{\partial x}$ where x is distance from the boundary into the cube.

$$c_p \frac{\partial T}{\partial t} - \left(-\nabla \cdot \kappa \frac{\partial T}{\partial x} \right) - Q = 0 \tag{8}$$

If we only ever had to deal with the conservation of energy in an infinitesimally small cube, we would be done. Let's stop and consider. This is the essential substance of the conservation of energy law. We can add more phenomena to the conservation of energy law such as phase transformations and make specific heat and thermal conductivity functions of temperature, microstructure and density. We can add velocity, i.e., stir the body if the body is a cup of coffee.

The basic idea remains invariant since it was proposed about 171 years ago by Joule in 1850. To learn how difficult it was for Joule to convince the world that conservation of

energy was a good idea, read:
https://royalsocietypublishing.org/doi/10.1098/rsta.2014.0348

For the ext step, let's divide and conquer, one step at a time. If we replace each little cube with a little finite element and then assemble the finite elements into a mesh to approximate a body or structure, we can deal with conductive heat flow in structures by solving the conservation of energy law in this set of elements using a finite element analysis algorithm or program. By the way, I have spent much of the last fifty years of my life designing and writing computer software to solve this problem of the conservation of energy in structures being welded in industry.

To solve this problem, we must integrate the conservation of energy over the finite element mesh in space and time. When we finish this second step, we are done with the conservation of energy, i.e., we have satisfied the conservation of energy as a constraint.

$$\int_\Omega \nabla \cdot \kappa \nabla T \, d\Omega = \int_\Gamma \kappa \nabla T \cdot \mathbf{n} \, d\Gamma \tag{9}$$

Note that the left hand integral is simply the sum of heat sources in the interior of the domain Ω. It is just a number. The right hand integral is the sum of thermal flux flowing through the boundary area Γ. It too is a number. The equation states that the two numbers are equal. We should mention that the temperature field must be smooth enough that the second derivative exist everywhere in the domain Ω. This equation is called the divergence equation or Gauss's equation.

We can do the differentiation in the above equation.

$$\int_\Omega \nabla\kappa \cdot \nabla T + \kappa \cdot \nabla^2 T \, d\Omega = \int_\Gamma \kappa \nabla T \cdot \mathbf{n} \, d\Gamma \tag{10}$$

Now rearrange terms in this equation.

$$\int_\Omega \kappa \cdot \nabla^2 T \, d\Omega = \int_\Gamma \kappa \nabla T \cdot \mathbf{n} \, d\Gamma - \int_\Omega \nabla\kappa \cdot \nabla T \, d\Omega \tag{11}$$

Conservation of Energy or Heat Equation in an Arc Weld. With specific enthalpy h, thermal flux q and a power density function Q, temperature T, temperature gradient ∇T, thermal conductivity tensor κ specific heat c_p, the heat equation can be be written in the following form:

$$\begin{aligned} \dot{h} + \nabla \cdot q + Q &= 0 \\ q &= -\kappa \nabla T \\ dh &= c_p \, dT. \end{aligned}$$

VrWeld solves this partial differential equation on a domain defined by an FEM mesh. The domain is dynamic in that it changes with each time step if filler metal is added to the weld pass. The initial condition is assumed to be a constant temperature usually of $300°K$. The material properties κ and c_p are temperature and microstructure dependent. The heating effect of the arc is often modelled by a double ellipsoid power density distribution that approximates the weld pool as measured from macro-graphs of the cross-section of several weld passes. A convection boundary condition $q = h(T - T_{amb})$ is applied to external surfaces. The FEM formulation of the heat equation leads to a system of ordinary differential equations that are integrated in time using a backward Euler integration scheme.

3.3. **Week 2: What stress, strain, deformation and elasticity really are.** Stress deals with the conservation of momentum, i.e., the balance of forces. Deformation and strain deals with the conservation of mass and the compatibility equation.

What is stress, strain and elasticity and what is a stress analysis of a structure from the viewpoint of computational continuum mechanics? For the past 100 years, stress and strain have been taught by solving problems in idealized linear elastic structures, usually beams and plates, largely based on theory and books written by Stephen Timoshenko. This was the best that could be done at the time. Now that finite element analysis codes and computers are available, it is better to gain a much deeper insight into continuum mechanics and solve nonlinear problems with arbitrary shapes. Computation crash analysis to optimize crash-worthiness in automobiles is a good example.

3.4. **Week 3: Fracture Mechanics.** Linear elastic fracture mechanics theory was developed largely from 1945 to 1975. It was driven by the failures of welded ships in World War II. This theory is currently embedded in regulatory codes for many industries such as nuclear reactors, power plants, pipelines, ships, bridges, buildings, aeroplanes, etc. It is used where ever a structure is at risk of failing due to the propagation of a crack, i.e., it is used to reduce the risk of failure by brittle or ductile fracture to socially acceptable levels.

This course will explain why Linear Elastic Fracture Mechanics (LEFM) theory as it is taught, presented and used today will soon become irrelevant and will no longer be used in industry or taught in engineering courses. Drafting was one of 5 full courses in first and in second year engineering in the 1950s. It was 2 of a total of 20 courses required for a B. Eng. degree at the time. Today, it is not taught at all. CAD has completely replaced drafting and CAD retains very few of the concepts that were taught in drafting. The mathematics of geometry has of course changed little in the past 2000 years but CAD has replaced the technology of drafting which is now irrelevant except for historians. (However, handling tolerances in a CAD system remains a hard problem because it is a hard problem.) Just as CAD replaced drafting, nonlinear computer models that model the nucleation and evolution of fractures that will be used by all designers, not just specialists in fracture mechanics, will replace Linear Elastic Fracture Mechanics (LEFM). The nonlinear models of fracture replace the complicated theories of Linear Elastic Fracture Mechanics (LEFM) with more general models of computational continuum mechanics.

3.5. **Week 4: Quality control, Taguchi methods, Design of Experiment (DOE), statistics, Response surface methodologies, Robust Design.** Quality control has existed since the stone age where people chose stones carefully. In the steel industry quality control reached a degree of maturity in the 1870s by applying chemistry to optimize steel making. In the 1950s Taguchi successfully introduced his concept for Design of Experiments (DOE) to industry with two critical novel ideas. Firstly he used orthogonal arrays that made it relatively easy for people in industry who were not experts in statistical analysis to design, set up and interpret results of an experimental Design of Experiment. This enabled relatively small companies to implement quality control based on sound statistical theory in their routine engineering design. Secondly, he included a loss function that tried to minimize the cost of the product to society. If a product has a short life or poor performance, this is a loss, not only to the customer, but also to society. Taguchi argued that an optimally designed product should have a long life, good performance and low cost to the customer to buy and to use. Today Taguchi's idea of a loss function is widely accepted because societies are concerned with climate change, sustainability and environmentally friendly products.

3.6. **Week 5: Optimization, Control Theory, FEM.** G. Strang said it best on page 666 in his book, Introduction to Applied Mathematics: *This chapter also completes the last of the three fundamental areas of applied mathematics: static problems, dynamic problems and optimization. There is no doubt that optimization requires the most finesse. It leads to the best design, while the others analyze a given design. In statics and dynamics the materials and the shapes and equations were given; now we have to find the equations before solving them. But the ideas are central to so many applications - old and new - that they belong in this book.*

At this time, my research team has the capability to analyze quickly, accurately and cheaply with high spatial and temporal resolution almost all of the welding problems in which the materials and the shapes and equations are given. The next goal of my research is to extend my research teams capability to solve weld optimization problems. In particular, to design optimal experiments for welding problems that have uncertainty and a stochastic dimension.

Distortion and residual stress involves deformation. It was not until 1970 that Ueda [10] did the first computation of residual stress in welds. From 1980 to 2000 CWM research evolved rapidly. From 2000 to the present, industry has been rapidly adopting CWM. In the author's judgment, current CWM software is designed to analyze a given problem with at most a few variations of parameters. Exactly in the sense that Strang said, current CWM software is not designed or implemented to support optimization. Of course, the capability to analyze a given design is an essential requirement for optimization. The important book [2], edited by Michelaris, describes the state of the art of techniques to minimize distortion and residual stress in welded structures in 2011. The fact that none of the examples in this book were solved by integrating formal computational optimization and CWM suggests that there is work to be done.

3.7. Week 6: Mid-term exam.

3.8. **Week 7: V&V Verification and Validation of computer models for design of mechanical systems.** In the 1980s and 1990s as computers began to be used routinely in industry in the decision making process for optimizing product designs and manufacturing processes, people began to ask to what extent should the predictions made by a computer model be trusted in making design decisions. To help decision makers seeking guidance on how they should answer this question, ASME published the standard for computer models for solid mechanics in 2006 and AWS published the standard for computer models for welds These standards propose concepts and procedures to i) verify, ii) validate computer models and iii) quantify the uncertainty in the predictions made by a computer model used in making a specific design decision. The validation procedure compares values of predictions made by a carefully designed computer model of the experiment with data measured in a carefully designed and executed experiment that is relevant to a specific design decision.

Experimental data should be verified by doing a Design of Experiments (DOE) to measure the uncertainty in data provided by experimental measurements. Experts in statistics recommend that 30 experiments be done to estimate a probable distribution function for the values of parameters in a design space. These experts also point out that no useful statistical data is provided by a single experiment. Authors of papers describing computer models of welds often rely on a single experiment and assume that the experimental data is sufficiently accurate that experimental error can be ignored. Rarely do papers published on computer models of welds provide data on the repeatability of experimental data.

3.9. **Week 8: Material science and material properties and behavior in design.** Material science is a vast subject. In this course, we will focus on low-alloy steels that are the material of choice for mechanical structure because of their low cost and because the strength can be controlled by varying the composition and the microstructure.

More than 80% of steel that is produced is welded. The microstructure in the Heat-Affected zone of the welds controls the maximum in-service performance of the welded structure. We will discuss the computer models of welds to optimize the microstructure in the design of welded structures that industry has begun to use

3.10. **Week 9: Fatigue.** Fatigue is the most common cause of in-service failures of mechanical structures. Current computer models to predict fatigue life usually are based on regression models that fit fatigue life to experimental data in which one fatigue test provides one data point. My team has recently developed a computer model to predict fatigue life for crack nucleation and fatigue life for crack propagation that is based on continuum mechanics. It computes a continuum function or field called damage that is defined at all points in the structure just as temperature, pressure, stress and strain can be defined at all points in a structure. This field can be correlated with measured data from fatigue experiments that can be gathered in each load cycle.

3.11. **Week 10: Creep.** Creep is an important cause of failures in structures that operate at high temperatures and pressures. Creep is viscous flow, i.e., the inverse or reciprocal of the viscosity times the viscous stress equals the the strain rate. This is an entirely different phenomena from the inverse of the elasticity tensor times the elastic stress equals elastic strain.

Corrosion is very important in design but it involves too much chemistry theory to be included in this course.

3.12. **Week 11: Shape Optimization.** Structural design problems can often be posed as optimization problems that minimize some function, often weight, subject to some constrains, e.g., the material is a low-alloy steel, the load, and the maximum deflection constrained to be less than some bound. A good example is designing a bridge over a given river for given loads. In the last twenty years, this has become important in aerospace and automotive design.

3.13. **Week 12: Global Optimization: Vector and Tensor Topology.**

3.14. **Week 13: Review.**