White Paper

# Modeling and Numerical Simulation

Supporting Innovation in Small and Medium Enterprises

Spring 2018
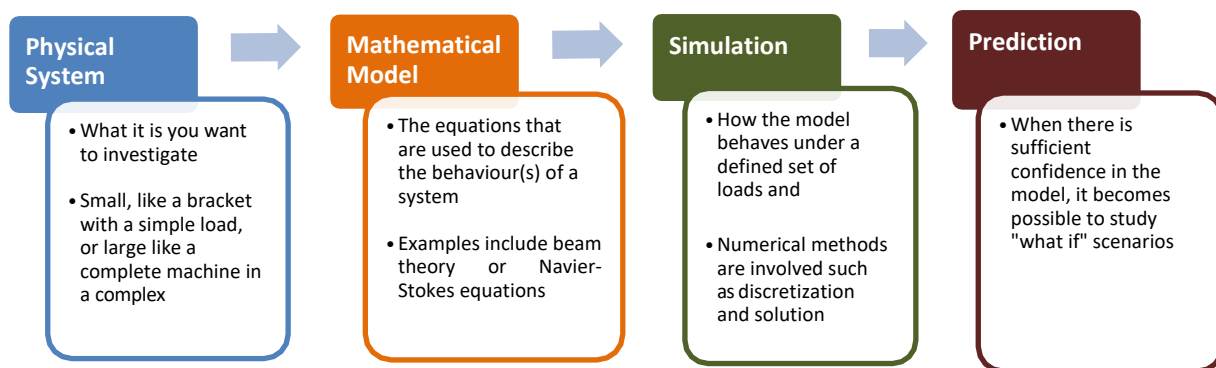
# Introduction

Finite Element Analysis? Computational Fluid Dynamics? Meshes? Material properties? High-performance computing ....... When it comes to modeling and numerical simulation, the number of tools available and their level of sophistication is enough to make the design engineer's head spin, let alone the folks on the project team with a less technical role.

So are these tools only for large companies? With a proper understanding of how these tools apply to your products or processes, it will become clear that modeling and simulation has the potential to support innovation in companies of all sizes, including Small and Medium Enterprises (SMEs). The goal needs to become smart users of the tools that are available. To achieve that goal, one has to understand some basic concepts.

# Definitions

The basic concepts need to be introduced so we can gain a common understanding and vocabulary. The vocabulary is introduced first and can be confusing initially; you may find that you need to come back as the discussion progresses.

**Physical System**
- What it is you want to investigate
- Small, like a bracket with a simple load, or large like a complete machine in a complex

**Mathematical Model**
- The equations that are used to describe the behaviour(s) of a system
- Examples include beam theory or Navier-Stokes equations

**Simulation**
- How the model behaves under a defined set of loads and
- Numerical methods are involved such as discretization and solution

**Prediction**
- When there is sufficient confidence in the model, it becomes possible to study "what if" scenarios

**Model**: Mathematical representation (object) that has the ability to predict the behaviour of a real system under a set of defined operating conditions and simplifying assumptions. Those mathematical representation are derived in a number of ways.

**Simulation**: The implementation of a model. It is the process of exercising a model for a particular instantiation of the system and specific set of inputs in order to predict the system response.

**Discretization:** The process of converting a continuous equation into a form that can be solved numerically.

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Prepared by Hubert Landry, PhD, PEng

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*Numerical Simulation* in engineering then implies that instead of trying to solve all equations for a problem in the entire problem domain, the problem is divided into smaller pieces (*discretization*), the smaller pieces are solved separately with methods like *Finite Elements* or *Finite Volumes*, and finally the partial results are put together to form the solution for the entire problem.

## What about hand calculations?

The topic of hand calculations allows us to clarify the "numerical" in numerical simulation. Analytical methods aim to find the exact solution to a mathematical model. For instance, beam deflection equations familiar to a lot of engineers are the result of an analytical development. For complex structures with complex loads, deriving exact analytical solutions becomes impractical if not impossible.

Numerical methods become necessary to tackle those more complex problems. The discussion on numerical methods can become quite involved, but there are two fundamental notions about numerical methods: (1) they provide an approximate solution, and (2) they require the discretization of the governing equations. Let's go back to calculus to illustrate the discretization concept. The continuous function that
describes the behaviour you want to study (the model) is integrated to calculate an answer. As you may

The model is $f(x) = y = x^2 + 3$ and we are interested in the value of its integral between x = 1 and x = 4.

The exact solution becomes $\int_1^4 f(x)dx = \int_1^4 (x^2 + 3)dx = [\frac{1}{3}x^3 + 3x]_1^4 = [\frac{1}{3}(4)^3 + 3(4)] - [\frac{1}{3}(1)^3 + 3(1)] = 30$.
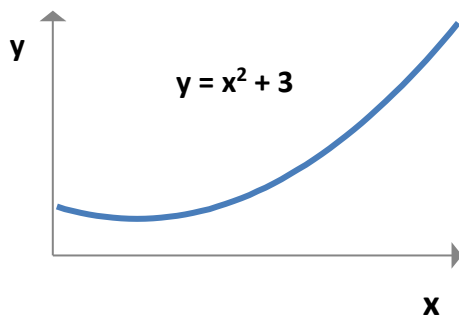


The exact solution represents the area under the curve. To find a numerical approximation, we can divide the interval of interest in sections, one section to start this simple case, and choose a simple function to approximate f(x) in that interval. Computers are good at solving large quantities of simple functions. The simplest function we can choose is a constant function that equals the value of f(x) at the mid-point of the interval. In this case, the constant function y = 9.25 is used as the function y(x) = 9.25 for x = 2.5. The product of this constant function and the length of the section approximates the integration of f(x) over that section. Here we have 9.25 x 3 = 27.75. When we further divide the interval of interest into 4

sections, still approximating the y-value of a segment to be equal to the y-value of the mid-point of that interval, we now have a total area of 29.859. By further dividing the interval into multiple sections, we can increase the accuracy of the calculation and move towards the true result of 30. That is what discretization is all about! For the more mathematically-inclined (i.e. geeks), what we have just described is the finite difference method of discretizing a differential equation.
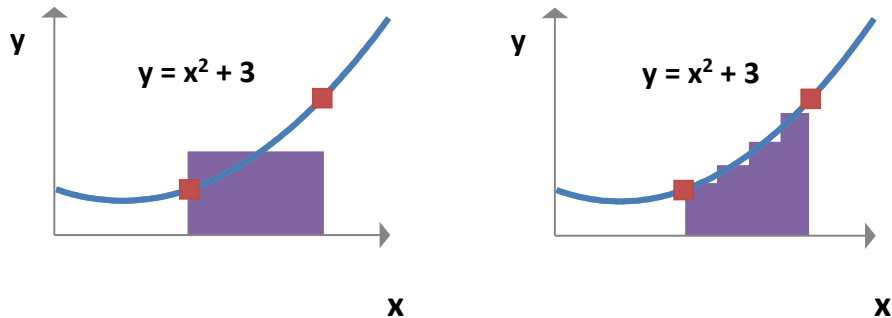


## Solids and structures need the Finite Element Method (FEM)

Hopefully we can start connecting some of the concepts here. The Finite Element Method (and we often hear about a Finite Element Analysis or FEA) is in essence the application of the numerical solving of the discretized physical and mathematical model. It is employed for solid mechanics and structural problems.  The key is to break down the real system (complex) into multiple smaller bodies or units (finite elements; elements that are finite in size in contrast to the continuum of the real system). The finite elements are interconnected at points called nodes. The nodes are the discrete points on the physical part where the analysis predicts the response of the part due to applied loading. All the elements form the finite element mesh and contain the material and structural properties of the model, defining how it will react to certain conditions.
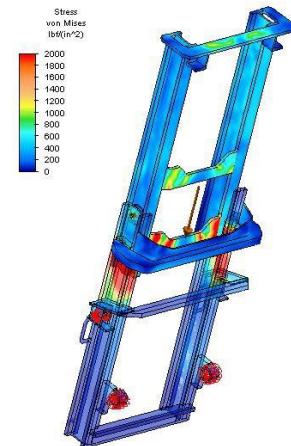


FEA has become an everyday tool that supports the design process. Linear FEA with static loads is frequently used and covers a broad range of the situations encountered by design engineers.  When larger deformation are involved, nonlinear analysis need to be performed to accurately predict the behaviour of the system.

When a structure deforms under load its stiffness changes.  Large deformations can also mean a  change in the shape of the structure. If the material reaches its failure point, the properties of the material change. The fundamental difference between a linear and a nonlinear analysis is the assumption that, when performing a linear analysis, the shape and material properties remain constant during the deformation process. The initial stiffness of the model is therefore maintained regardless of the stress levels that develop in response to the applied load. The basic matrix equation [F] = [K] x [d], involving the known vector of nodal loads [F], the known stiffness matrix [K], and the unknown vector of

displacements [d], contains a very large number of algebraic equations. The stiffness matrix depends on the geometry, material properties and constraints. When performing a linear analysis, the model stiffness is considered constant and the set of equations only needs to be assembled and solved once as a result. That is why linear analyses require much less computational resources when compared to nonlinear analyses.

When performing a nonlinear analysis, the assumption of constant stiffness is no longer used and the stiffness matrix needs constant updating as the nonlinear solver iteratively works towards a solution. The iterative process takes much longer than the straight path of the linear analysis. There are a number of reasons to resort to the nonlinear approach. The geometry of the problem may cause nonlinearity like when deformation is expected under operating loads. Also, some materials exhibit nonlinear behaviour, with rubber as a prime example of such a material. Nonlinearity can also come from contact and support conditions.

> The big warning here is that observing nonlinear behaviour (large deformation or stress levels suggesting yielding) when performing a linear analysis invalidates the results of the analysis.

What about dynamic analysis? Well, a dynamic analysis takes into account inertial effects, damping, and time-dependent loads. Vibration or impact analyses are examples of dynamic scenarios. A dynamic analysis can be linear or nonlinear, using the exact same discriminating factors as the non-dynamic analysis. Crash simulation or metal stamping modeling require nonlinear dynamic analysis because they deal with both large deformations (nonlinear geometry) and large strains (nonlinear materials).

## Fluid flows call for Computational Fluid Dynamics

Fluid flows are governed by partial differential equations (PDEs) that represent conservation laws for the mass, momentum and energy (the mathematical model). The CFD method consists of replacing the system of PDEs by a set of algebraic equations which can be solved numerically by a computer. Sounds familiar? So the same process of approximating the governing equations by simple functions applies, followed by the division of the domain in smaller units (discretization) so that the equations can be solved numerically using initial and boundary conditions. The physical phenomena involved in fluid flow are complex and nonlinear so an iterative solution approach is required.
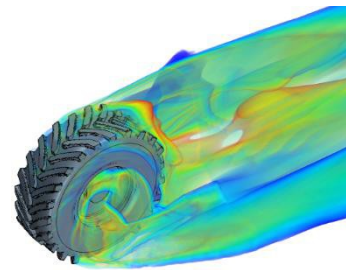
## Particle flows are solved with the Discrete Element Method

For granular and discontinuous materials, the best approach is to use the discrete element method (DEM), a numerical method for computing the motion of large numbers of particles. The great divide here is the discontinuous nature of the system (powder, soil, grains, etc.).
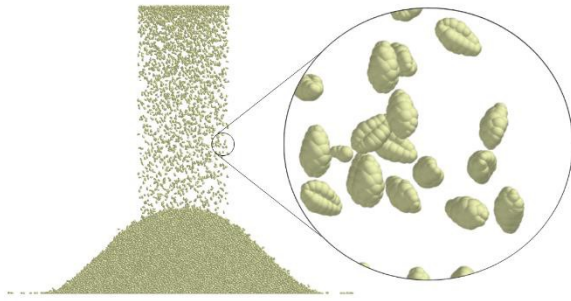
DEM considers a system as a collection of discrete entities; this is in contrast to the Finite Element Method (FEM) which treats a bulk particulate system as a continuum. Therefore DEM provides knowledge of the particle behaviour at the scale, enabling a better prediction and understanding of the macro scale (the bulk system). DEM calculates the sum of the forces acting on the particles and integrates Newton's equation of motion to obtain velocity and position at the next time step. In doing so, the DEM describes the path of every particle in the assembly as time proceeds. The DEM is all about contacts and collisions (particles with particles as well as particles with the physical domain); the time-stepping algorithm used to generate the solution is very computationally

## Rigid Body Dynamics (RBD)

Rigid body dynamics simulations are concerned with the movement of systems of interconnected bodies under the action of external forces. Because the bodies are considered rigid, they do not deform during the simulation which simplifies the simulation. Collisions are however important as they can impact how the system behaves. The simulation requires solving the equations of motion that are formulated from information on each rigid body (mass, center of mass, inertia tensor) and interaction conditions between bodies (forces, constraints). The name multibody dynamics (MBD) is often seen, and it generally implies going beyond the motion and interactions of rigid bodies to include actuation and control. The loads generated by an MBD analysis can be used in an FEA. That leads use to our next section on combining various methods.



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## Multiphysics systems

In industry, a large proportion of systems involved more than one physical phenomenon.  A relatively recent trend in the world of numerical simulations is the coupling of two (and sometimes multiple) methods. The simple form of a multiphysics analysis is done by doing sequential simulations when the output of one analysis informs the following analysis in the form of initial or boundary conditions. More often than not, the physical phenomena are strongly coupled requiring concurrent simulations that exchange data on the go.  The system of interest may involve the movement of particles in air as in

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pneumatic conveying in which case, a coupled DEM-CFD approach may be appropriate. The field of fluid-structure interactions (FSI) has also emerged, where the interest is in the loading and deformation of structures as influenced by fluid flows.  In turn, the flow fields may change as a result of the displacement or deformation of the structure. Heat generation and cooling applications are also examples of multiphysics problems.

# The process for modeling and simulating a

The process of analyzing a system generally requires a number of steps.

## Understanding the system

This step is primarily about defining the scope of the analysis. Resources are always limited, whether engineering time or computing power, so it is important to properly define the scope of the analysis.  With the sophistication levels of commercial software, it is tempting to include too many details that may or may not be relevant. One golden rule is to start simple and build up.

## Geometry simplification

Most companies operate in a CAD-centric universe meaning that the model will be rooted in a CAD environment and will need to migrate to the simulation code. A number of CAD features need to be removed to make the simulation more efficient.  That step is sometimes called cleaning up or defeaturing the CAD model.  Small CAD details and intricate geometries will make the meshing step more difficult and should be removed. Also, fasteners are generally not required for most analyses. One has to be careful however as small features like fillets can greatly influence the results of a stress analysis. The simplification must take into account the intent of the analysis.

## Meshing

As we now know, meshing is required to spatially discretize the system under investigation. The number, size and type of elements are all important and related to what the information of interest is.  For instance, studying bending using solid elements requires that several elements are generated through the thickness of the part; in some cases that makes the number of elements prohibitively large. Shell elements can be a good alternative but parts connectivity may become a challenge and require modifying the geometry of the model significantly. Meshing is also done strategically with the intent of the analysis in mind.

## Applying appropriate loads, boundary conditions, and material properties

This step is intimately related to the understanding of the system that was developed at the beginning of the analysis. The model will likely have been simplified, introducing loads and / or boundary conditions that must be adequately accounted for during the simulation. It can be quite advantageous to replace the actual pin in a model by a pin boundary conditions.  When restraining a part, one has to consider what the true constraints are (rotation or translation, in which direction) and understand how these constraints

can impact the results. It can be quite acceptable to over-constrain an edge or a surface, but understanding how this may impact the behaviour of the model and the results of the simulation is important. Lastly, the properties of the materials have to be selected to properly represent the real system. Also, it is important to recognize that two categories of properties are generally required: properties that will allow calculating the response of the material and properties that will impact how the response is interpreted or will evolve, or failure properties.
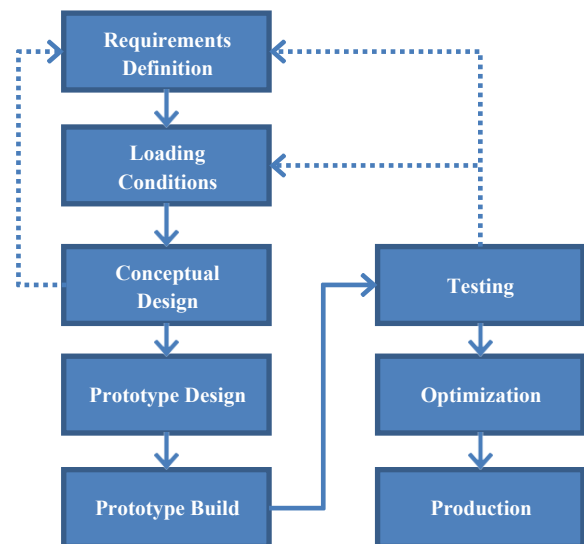
**Interpreting the results**

As eluded in the previous steps, the results of a simulation must ALWAYS be interpreted in their entire context. Knowing what simplifications were made on how they may impact the results is paramount to interpreting what results the simulation yielded.

# Is it for the designer or the

Well, ideally, you would use a team approach where analysts work side-by-side with your design engineers to get the most out of any modeling and simulation exercise. The sophistication and ease of use of today's commercial software packages is both a tremendous advantage and something that invites caution. Unless routine use is made of a simulation code, it can be difficult to proficiently set up and run simulations given the multitude of options and settings available. The team must be cognisant of its own limitations, start simple and build up. It is important to match the complexity of the model with the information that is sought. The design engineers can provide exceptional value in applying their knowledge of the system to the results provided by the analysts. Both the analyst and the designer will benefit for the insights provided by M&S into the failure mode(s) of the system.

# Role in the innovation

To illustrate how modeling and simulation can benefit the innovation process, let's look at one embodiment of the design process. At the beginning of the design process, the requirements of the system or process are defined including what its performance requirements are and what environment it must work
in. Form that set of requirements, some or all of the internal and external loads may be determined. At that point, it is possible to develop a high-level design of what components or sub-systems may be able to meet the requirements. There may be a need to iterate between the conceptual design and the

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When the conceptual design has reached a sufficient level of details, it has become the prototype design that can be built or implemented. At that point a testing regime can be contemplated and with test results, the design can be improved or optimize to finally reach a level that satisfies production requirements. Now let's look at where modeling and simulation can be used in the design cycle.

During the requirements definition stage, M&S can be used to determine loading conditions. An but very relevant example is the determination of the loads that a vehicle protection system needs to sustain in a blast event. Hand calculations or the experience of the design team may not be sufficient to quantify those loads. M&S become an important tool to evaluate conceptual designs before any drawings hit the shop floor. The most common use of M&S is probably as a complement to physical testing. M&S can indeed streamline the testing phase and reduce its cost by studying a number of what-if scenarios ahead of testing. The test matrix can therefore be optimized to generate the most useful data. Finally, M&S can contribute to the optimization of the system by supporting the investigation of potential modifications as informed by the test data available. One could argue that M&S can also play a role in the production aspect in terms of materials selection, flow of manufacturing tasks and other aspects.
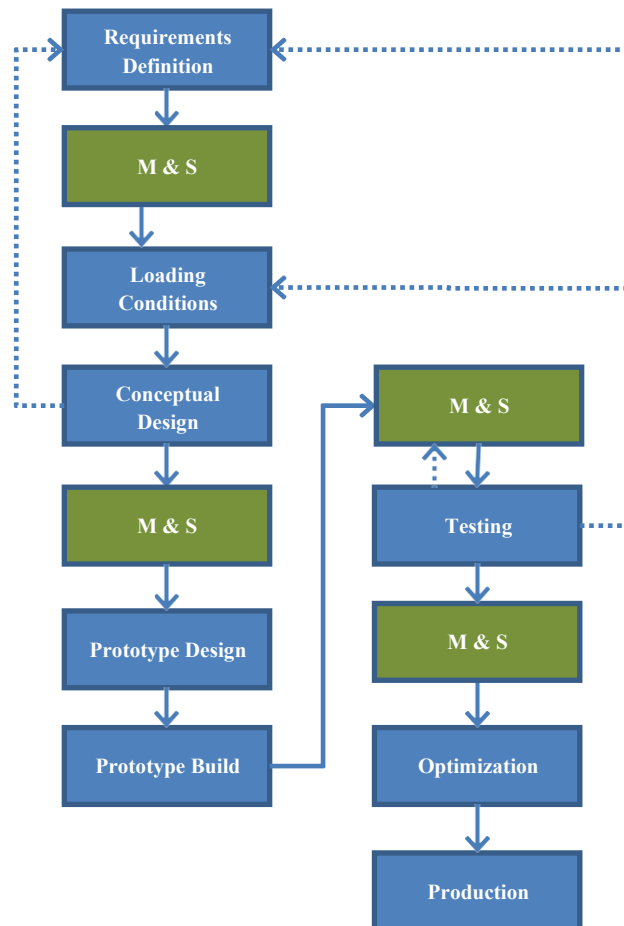
## Conclusion

In summary, modeling and simulation is a powerful tool that allows engineers to better understand product performance, achieve optimized designs faster, and release products to market earlier. You may have heard the expression "fail fast, fail cheap"; let's add "fail fast, fail cheap, and fail on screen". The aspect of risk management is also key in assessing the usefulness of modeling and simulation. Understanding failure is paramount to managing risk from safety, to warranty aspects, and even to provide guidance for future research and development efforts. With a good understanding of what modeling and simulation can achieve and the right partnerships as appropriate, SMEs can greatly benefit from these tools.

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