Multiphysics Simulation Applications

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Abstract: A series of multiphysics Simulation Applications have been developed to address a range of complex physical phenomena. The Simulation Applications were developed using COMSOL Multiphysics® and have been supplemented with additional software control functions integrated with COMSOL Server™ to enable routine, distributed use on high performance computing hardware.

Keywords: Multiphysics, Simulation applications, High performance computing

1. Introduction

Increasing demand for new technology, products and processes to provide improved performance, achieve proof of concept, offer higher quality and meet demands for on-time and on-budget delivery have put increasing pressure on scientist and engineers to predict performance before physical prototypes are built and tested. To address these demands, more focus has been placed on the use of predictive physics based computational models to provide information with limited physical prototypes and enable rapid iteration of designs. The benefits of virtual prototyping have been well documented by a number of industry studies, for example Figure 1.

Figure 1. Key metrics associated with physical and virtual prototype development, Aberdeen Group, 2014

The increased demand for computational modelling is no longer restricted to large multi-national corporations and is being rapidly adopted by small and medium sized enterprises who are seeking to innovate and differentiate themselves from their competition. In addition, large companies are seeking to cascade routine use of computational modelling onto engineers with limited or no familiarity with computational analysis. This trend has recently been labeled by many sources as "democratization of numerical analysis".

The increasingly limited availability of expertise to perform computational analysis, means that routine use of computational analysis requires more streamlined access with simplified interfaces for analysis of predefined problems. Developments of this type will allow design and process engineers to perform a series of analyses easily and use the results to aid decisions on developments without having to make direct use of computational analysis domain experts. This approach has recently become a viable option through the release of capability to allow the development and distribution of packaged Simulation Applications.

To address critical areas of commercial relevance AltaSim has developed a series of Simulation Applications using the Application Builder capability in COMSOL Multiphysics®. These Simulation Applications solve multiphysics-based problems and allow the non-expert user to investigate the solutions to a range of complex multiphysics-based technologies. To expand the effectiveness of these Simulation Applications and increase the complexity of problem they can address, access to increased computational hardware is often needed. Integration of this capability provides an additional level of complexity that can hinder even the most skilled computational analysis expert. In this work, intelligent decision-making algorithms that automatically distribute problem solving across distributed memory systems have been integrated into the multiphysics-based Simulation Application solution methodology. In this way, the complexity of performing both multiphysics-based analysis and the intricacy of running analyses on large scale computing resources have been overcome thus allowing routine use by personnel with limited expertise in computational analysis and high-performance computing (HPC) resources.

2. Computational analysis

Multiphysics-based Simulation Applications are designed to be used by the large group of personnel with limited or no experience in computational analysis and yet must contain the complexity and knowledge of simulation and domain experts to ensure accuracy and efficiency. Underlying any multiphysics-based Simulation Application is the COMSOL Multiphysics® computational analysis that is driven by a simplified Graphical User Interface controlled by the user. The complexity of formulating the problem, controlling meshing parameters, assembling the physics, ensuring a converged, accurate solution is reliably obtained and control of post processing functions for display of relevant results is hidden from the user.

Here the structured development of multiphysics-based Simulation Applications with complex functionality is demonstrated with respect to two practical problems of current commercial interest, namely:

1. Design of heat sinks for electronic control circuits - HeatSinkSIM™, and
2. Simulation of powder bed fusion (PBF) additive manufacturing (AM) - AMThermSIM™

2.1 Governing Equations

Both AMThermSIM™ and HeatSinkSIM™ consider the effects of heat transfer due to conduction, convection and radiation to the surrounding media. Conduction within the solid and liquid part are described by the standard heat equation:

$$\rho\, c_p \frac{\partial T}{\partial t} = \nabla \cdot \left(\lambda \nabla T\right) \tag{1}$$

Here, ρ is the density of the solid material, c_p is the specific heat capacity, T is the temperature, and λ is the thermal conductivity. The density, specific heat capacity, and thermal conductivity are functions of temperature.

The heat flux at the surface of the part due to radiation is modeled as:

$$q_r = \varepsilon_{emis}\left(G_m + F_{amb}\sigma\, T_{amb}^4 - \sigma\, T^4\right) \tag{2}$$

where ε_{emis} is the emissivity of the surface, G_m is the mutual irradiation from other surfaces, F_{amb} is the ambient view factor, σ is the Stefan-Boltzmann constant, T_{amb} is the far-field ambient temperature, and T is the temperature at the surface. G_m is a function of the radiosity J, which is the sum of the emitted heat flux and the reflected heat flux and is given by the following equation:

$$J = \left(1 - \varepsilon_{emis}\right)\left(G_m + F_{amb}\sigma\, T_{amb}^4\right) + \varepsilon_{emis}\sigma\, T^4 \tag{3}$$

Any temperature-dependent emissivity is based on published information. If mutually irradiating surfaces are present, ambient view factor and mutual irradiation are automatically calculated. In the case of no nearby radiating or reflecting surfaces, the radiative heat flux reduces to:

$$q_r = \varepsilon_{emis}\sigma\left(T_{amb}^4 - T^4\right) \tag{4}$$

For the analysis of the heat sink, fluid flow is modeled subject to the physics described by the conservation of mass, momentum, and energy according to the following equations:

$$\nabla \cdot \left(\rho\, \mathbf{u}\right) = 0 \tag{5}$$

$$\rho\, \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left(\eta\left(\nabla \mathbf{u} + \left(\nabla \mathbf{u}\right)^T\right) - \frac{2}{3}\eta\left(\nabla \cdot \mathbf{u}\right)\mathbf{I}\right) + \rho\, \mathbf{g} \tag{6}$$

$$\nabla \cdot \left(-k \nabla T\right) = Q - \rho\, c_p \mathbf{u} \tag{7}$$

The viscous heating and pressure work terms are neglected in the energy equation. In the above equations, ρ is the density, $\mathbf{u}$ is the velocity vector, p is the pressure, η is the dynamic viscosity, $\mathbf{g}$ is the gravitational acceleration vector, k is the thermal conductivity, T is the temperature, Q is a heat source term, and c_p is the specific heat capacity. The viscosity, thermal conductivity, and specific heat capacity are functions of temperature, while the density is a function of both temperature and pressure.

For analysis of the PBF AM process, a moving thermal source due to the laser beam is applied with additional heat sources incorporated due to temperature dependent material phase changes between solid-liquid-solid and also solid-state phase transformations. These additional heat sources are integrated into the thermal model using standard representative material temperature dependent material properties.

3. Simulation Applications

Development of Simulation Applications can be easily performed using the Application Builder functionality in COMSOL Multiphysics®.

3.1 Preliminary App Development

In the initial work, the Simulation Applications were designed to run on standard desktop computer systems. For analysis of the PBF AM processing, the Simulation Application interface (AMThermSIM™) allows the user to develop simple geometries and select representative operating conditions for use with controlled laboratory-based AM systems, Figure 2.

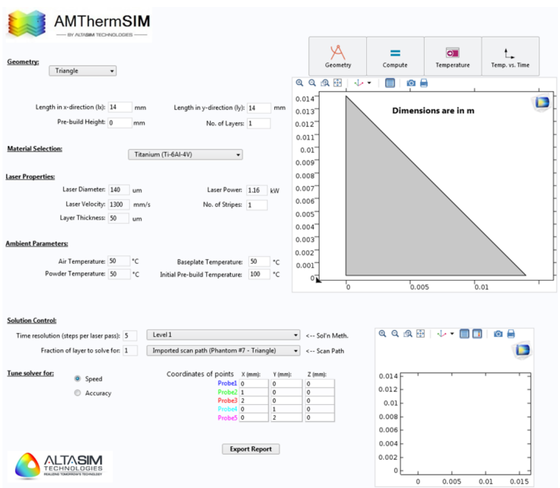

Figure 2. Initial user interface of AMThermSIM™ for analysis of PBF AM.

Based on successful use of the initial version of AMThermSIM™ further extension was required to provide analysis of commercial PBF machine control. This requires that the user have the ability to import complex component geometries defined by standard CAD files and define the AM processing by importing AM machine control parameters, e.g. Figure 3.

Similarly, the initial version of HeatSinkSIM™ was extended to include parametric sweeps over a range of design and operating parameters to allow the import of complex geometries of the heatsink and enable the optimum design of a heatsink to be automatically predicted.

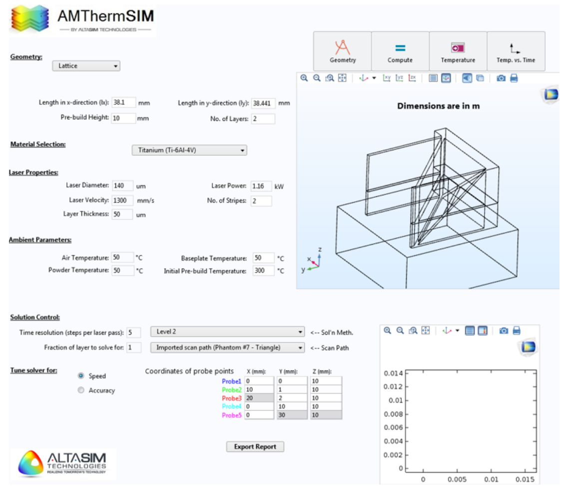

Figure 3. Import of complex geometry for analysis of PBF AM.

3.2 Enhanced App Functionality

The enhanced functionality added to AMThermSIM™ and HeatSinkSIM™ required the use of computational hardware with increased resources. In addition, extension to addressing practical product and process design issues necessitated use by multiple engineers. The increased functionality, complexity and requirements for access led to the need to:

1. Enable access and use by multiple users on a centralized computer system, and
2. Automate App usage on HPC resources

Providing access to multiple users is accomplished through use of COMSOL Server™. This allows users to run the Apps using:

1. A web browser
2. COMSOL Client

With either method, the user then accesses the App from the Application Library to which they have been provided with access.

COMSOL Server™ also allows use on Cluster computing hardware systems, providing automated distribution over available nodes/cores. However, for use of the Applications described here, a further level of customization was required such that the analyses can be submitted to a scheduling system that keeps track of the current state of all resources and jobs and decides, based on conditions, policies and availability, where and when to start jobs.

In this case, submission of jobs is non-trivial for even the most experienced of computational analysis experts. Under circumstances where the Apps are expected to be run by personnel with limited or no experience in computational analysis the impact of the barrier to execution is magnified.

To overcome this barrier, additional control scripting was developed to interface between the scheduling system and COMSOL Server™. The user accesses and sets up the analysis directly using the COMSOL Server™ functionality. Once the scope of the problem is defined, the control script identifies the problem size, estimates the memory requirements, identifies the most efficient combination of RAM/nodes/cores available on the system that is suitable for the required analysis and submits the job the scheduling system for execution. Once complete the user is notified of the location of the results for subsequent download and inspection. In this way, both the complexity of developing the relevant computational analysis file and performing the analysis on HPC facilities is removed from the user's responsibility and the user is interacting with a single, simplified interface.

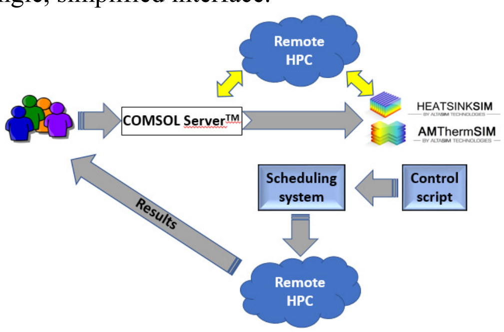

Figure 5. Process for App submission, execution of multiphysics-based analysis and retrieval of results.

4. Summary

An integrated approach has been developed and deployed to allow engineers who have no knowledge of multiphysics-based computational analysis, to perform complex analyses. The approach combines the specialized functionality of the Application Builder in COMSOL Multiphysics®, COMSOL Server™ with supplemental software for computer system control, to provide an environment that allows engineers to develop and execute multiphysics-based analyses for the design of additive manufacturing processing technology and cooling of microelectronic process control equipment.