THESEUS-FE 5.0

major version 5.0 arrives with numerous improvements on board
- improved numerical solver with parallel computation facilities
- new module for simulating the E-Coating process of a body-in-white
- enhanced optimization methods for parameter calibration and sensitivity analysis
- refracting media for modeling optical media like glass lenses in headlights
- and many, many more…
Arrival of major release version 5.0

In march 2015 our latest major release 5 arrived with plenty of new features and even whole new modules on board.

The major advances in the THESEUS-FE portfolio are the new E-Coating module for simulating the electrophoresis process of a body-in-white in a paint bath and a completely overhauled parallel numerical solver. Of course, these two major topics are not the only amendments and improvements in THESEUS-FE. The most mentionable ones are either presented in further detail in this newsletter or shortly noted in the following short list of changes in solver and GUI. But altogether they are only a small fraction of the work that has been incorporated in version 5. For everyone interested in the fine-grain changes in version 5 that have been made since the last major version, please have a deeper look at the release notes accompanying each release package.

The changes to the numerical solver that are most worthy of mention are:
- completely overhauled parallel solver with noticeably reduced computation times
- utilization of multi-core processors in nearly all time-consuming portions of the solver (e.g. view factor calculation, solar load calculation, FEM system assembly and solving)
- radiation model for refracting and absorbing media which enables modelling of optical lenses for thermal headlight simulations for example
- anisotropic heat conduction for solid elements
- upstream concept for defining the flow between volume and airzone objects in a more convenient manner
- enhancements and additions to the TISC coupling interface

For the graphical user interface (GUI) users should have a look at the following new features:
- several new convenient tools like a result calculator and hardening calculator for Oven simulations
- support for importing thermal ABAQUS models
- user-defined views can be stored and re-imported to support a standardized post-processing workflow
- visualization of ray data generated by the solver during ray tracing for short-wave radiation
- several improvements for easier handling of simulation models in pre- and post-processing

The co-simulation tool THESEUS-FE Coupler has been extended with several new features as well:
- support for OpenFOAM 2.2.x and 2.3.x
- support for Flowmaster 7.9.2
- steam transport for OpenFOAM solver
- increased robustness of data communication with OpenFOAM through using a TCP/IP connection
- additional tutorial case for cabin cool-down simulation using Star-CCM+
- improved process for coupling the FIALA-FE human comfort manikin with Star-CCM+ simulations

The THESEUS-FE Optimizer has undergone a major overhaul and comes packaged with
- a new streamlined keyword for the existing genetic algorithm for clearer set up of algorithm options
- new derivative-free optimization algorithms (Hooke-Jeeves and Nelder-Mead) for finding the optimal model parameters more quickly and with greatly reduced computational effort
- improved parameter study methods with more suitable patterns of function evaluations
- support for the MS-MPI v5 distribution on Windows platforms for robust setup of optimization analysis

Miscellaneous:
- a new comprehensive database of thermal material properties is included in the installation package
Parallel solver: substantial reduction of solution times for large models

The typical size of finite element models used in THESEUS-FE simulations is ever increasing from year to year. Understandably, our users request for models that are as detailed as possible to improve the accuracy of their simulation results. Together with the ongoing trend in modern computer processor architectures for a steadily increasing number of execution cores per processor this led to the demand to lift THESEUS-FE into the parallel computation age. During the last year, large parts of the THESEUS-FE solver have been completely overhauled and existing serial algorithms have been replaced by scalable parallel algorithms as widely as possible.

While small to medium sized models benefit from our work quite decently, especially large and huge models consisting of several thousand of elements benefit quite heavily from the new parallel algorithms. Besides the core numerical equation system solver, also the view factor and solar load calculation have already been parallelized as well. The remaining parts of the solver which are still working solely in serial mode (mainly a few parts in pre- and post-processing) will be reworked within the next several months. The scalability of THESEUS-FE simulations will thus further improve with each new upcoming release.

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<tr>
<th>Thermal Vehicle Cabin Simulation</th>
<th>Paint-Dryer Simulation (OVEN module)</th>
<th>E-Coating Simulation</th>
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<td><strong>Solver</strong>: CG with ILU0</td>
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<td><strong>Comparison of simulation times using the new parallel solver for models in some typical application areas</strong>&lt;br&gt;(benchmark machine: HP Z420, Intel Xeon E5-1620 v2 @ 3.60 GHz, 32 GB DDR3 RAM)</td>
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Parallel solver: new token-based licensing scheme for parallel simulations

With the new parallel solver we are introducing parallel solver tokens as a new license feature. Introducing this new licensing feature allows our users to tailor their licenses to their own simulation needs. Parallel simulations with THESEUS-FE will require a varying number of so-called parallel tokens based on the number of cores participating in the parallel analysis. We tried to keep the number of necessary parallel tokens and their pricing as fair as possible. Users with an existing license of the Advanced package of THESEUS-FE will receive one parallel token free of charge. Oven and E-Coating packages will come bundled with 6 parallel tokens to allow simulations on up to 8 cores. This should allow nearly all users to try out the parallel solver and judge its benefit for themselves. For additional questions regarding parallel simulations and their licensing, please get in touch with us or your local sales representative.

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<td>C = # of cores in parallel analysis</td>
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**Number of parallel tokens required for parallel analyses**

C = # of cores 1 2 3 4 5 6 7 8 16 32
N_{PT} = # of parallel tokens 0 1 2 3 4 5 6 7 8 16
BACKGROUND – MOTIVATION

THESEUS-FE version 5.0 includes the new E-Coating module to simulate typical electrochemical painting processes in the automotive industry. The development and validation of the new simulation technique took place in collaboration with the Volkswagen Paint Planning Department in the last two years. Today we are ready for the market, and offer a specialized graphical interface and our new parallelized solver for rapid and precise e-coating quality predictions. The E-Coating module is part of our strategy of offering simulation capability covering the entire automotive coating process during production. Using this technology we can offer results for the e-coat layer thickness and uniformity. This is complemented by our Oven module where we predict temperatures in the paint drying ovens that are used in the following production phases.

BASIC PRINCIPLES

Cathodic deposition coating is the current state-of-the-art technique used in the automotive industry for applying anti-corrosion layers to car bodies-in-white. After pre-treatment such as cleaning and phosphate coating the car body is dipped into a paint bath. An electric voltage of approx. 300 V DC is applied between the car body acting as cathode and a series of stationary anodes along the bath walls. The resulting electric field causes a migration of the ionized paint particles in the solution towards the car body. At the car body chemical reactions take place and the paint particles precipitate out of the solution to form a coat layer on the body. The increasing coat layer thickness results in a locally higher electric resistivity, which in turn causes the electric field to bend around the already coated surfaces to seek paths of less resistance. This self-regulating behaviour, known as throw-power, creates a uniform coat layer with a thickness ranging between 5 to 30 microns.

For a simulation of the paint layer thickness the user needs to supply a handful of paint and process parameters, including the conductivity of the paint solution and deposited layer, the electrochemical equivalent, and the anode voltage over time as felt by the moving body. The THESEUS-FE E-Coating GUI accepts the usual Nastran FE format as import. Setting up an E-Coating simulation is then a matter of minutes, with full visual feedback for the model definitions available at any time.

The solver accepts the finished e-coating model and produces a solution for the coupled electrostatic field problem and transient paint layer thickness evolution equation. Typical runs on multicore workstations with full body geometries are typically done in a matter of hours. Since some of the process parameters, especially the solid paint layer conductivity, are not easily measured, our Optimizer module is regularly employed in practice to calibrate the model against measurements of paint thicknesses. Recalibration of the model is only necessary for large-scale changes of paint chemistry or initial runs for new plants.

Success stories

Our partners at Volkswagen helped us carry out extensive validation work for the new module. As an example we cite a comparison of predicted and measured coat thickness in the interior of a vehicle column, see the following page. With recent advances in the meshing procedure and solver speed gains due to parallelization an experienced engineer can create E-Coating models and results starting from CAD geometry within a matter of days. For calibrated paint baths the maximal overall error for the predicted paint layer thickness is typically in the range of 2-3 microns, thus approaching the tolerance of the measurement equipment.

At the moment Volkswagen runs every new vehicle model through the THESEUS-FE E-Coating simulation process, with further rollouts at other brands planned in the near future. Other major OEMs rely on our engineering consultancy services for E-Coating simulation.

Comprehensive database of thermal material properties

Our new release comes bundled with an all-new material database containing thermal properties for several hundred materials. Values for the specific heat, density and thermal conductivity are given – for many of the included materials even for a wide range of temperature values. Numerous common materials are listed, for example a vast number of metals, plastics, foams and other frequently used organic and inorganic materials.

With this material database the search time for suitable material properties during the setup stage of creating any analysis model for THESEUS-FE can considerably be reduced. Where searching for certain material properties could be a task of several hours in the past it can now be achieved within a few minutes only.
Further improved modelling of headlights

With the implementation of refracting and absorbing media in version 5.0 of THESEUS-FE, many simulations including transparent components can now be modeled even more realistically leading to considerably more accurate simulation results. One major application area of THESEUS-FE where this is highly beneficial is the thermal simulation of automotive headlights. These very often comprise sophisticated lens systems which obviously must not be neglected when analyzing the light and thermal energy transport inside the headlight.

A completely revised tutorial case demonstrates the new key modeling techniques for treating headlights with optical lenses.

New Optimization and parameter study methods

The THESEUS-FE package includes a specialized optimization tool for optimizing model parameters of an input deck. For E-Coating models the model parameters in question are typically the electrical conductivity of the liquid and dried paint for example. These quantities vary strongly based on the voltage applied at the anodes as well as the temperature that arises in the paint bath and near the body-in-white. The electrical conductivity is strongly dependent on the whole history of conditions during the paint layer forming (voltage, electric current, temperature). Often the proper model parameters can not be determined through simple measurements but have to be fit using measured results and can then be re-applied in E-Coating simulations of various car body types. In Oven simulations the model parameters in question are typically the temperatures of nozzle heat streams, their length of effect and the heat transfer coefficients they result in at the car body. In the past, the only optimization algorithm available in the THESEUS-FE Optimizer was based on a genetic algorithm. While still applicable for many optimization tasks, the drawback of this method is the demand for a huge amount of simulations especially in cases, where several model parameters have to be determined simultaneously. This demands for high computational power for such kind of parameter calibrations which can sometimes lead to several days of computation time. The latest installment 5.0 of THESEUS-FE provides two new optimization methods that are able to find the optimal parameter values with considerably less computational effort. These are the pattern-search-based Hooke-Jeeves method and the amoeba-based Nelder-Mead method.

Modelling of dryer section with non-moving body-in-white with stationary Oven nozzles

Stationary nozzles may now be defined in Oven models. The intent of this nozzle variant is to model sectors in a paint dryer where the car body remains stationary for a certain period of time. The classical nozzle model combines several individual nozzles on the same side in the same height into a single line. This is perfectly suited for the usual sections in a paint dryer where the body-in-white is moving along with a certain velocity. In such sections, individual nozzles do not affect the temperatures of the simulation model in a distinct localized manner but typically result in elongated patterns along the whole car body side. The new nozzle variant is modelled by individual cone-shaped areas of effect for every single nozzle in the paint dryer. This is only suited for periods, where the car body is not moving at all and will result in strictly localized areas of effect. The picture nearby shows a typical Oven model with the application and impact of such stationary nozzles.
Publicly funded BMBF project E-comfort has successfully been completed

In June 2014 the THESEUS-FE group concluded its work on the government-funded project E-Komfort. In the project consortium comprising Volkswagen, Fraunhofer Institute, RWTH Aachen, and P+Z Engineering our contribution consisted of developing innovative techniques for cabin AC and comfort simulation geared towards electric vehicles – in this case the platform under focus was the new Volkswagen E-Golf 7. It is well known in the community that battery-driven electric vehicles pose new challenges to AC design. Traditional approaches for ICE-driven vehicles rely on the easily accessible mechanical energy available from the engine for powering the AC system. In addition to that, the heating system can make use of the waste heat from the motor for directly heating the cabin.

Battery-driven electric vehicles must sacrifice valuable electrically stored energy for air conditioning – in many circumstances the price for this is reduced vehicle range. New and innovative techniques such as zonal AC, local heating and cooling technology, and passive concepts such as solar energy panels for ventilation during standby are necessary to conserve battery power.

THESEUS-FE was used together with OpenFOAM to provide valuable insights by means of coupled CFD/thermal cabin simulations. The THESEUS-FE Coupler module was developed in the course of the project to allow robust and user-friendly setup and execution of co-simulation scenarios.

Click here for further information on our website

VW e-Golf: reality and the THESEUS-FE simulation model (cross-section)

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