Thermal Modelling of a Fragrance Extraction Reactor in the Cloud with COMSOL Multiphysics

An UberCloud / ForCES Cloud Experiment

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CPU 24|7

UberCloud

UberCloud Case Study 192

http://www.TheUberCloud.com

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Welcome!

The UberCloud** Experiment started July 2012, with a discussion about cloud adoption in technical computing and a list of technical and cloud computing challenges and potential solutions. We decided to explore these challenges further, hands-on, and the idea of the UberCloud Experiment was born, also due to the excellent support from INTEL generously sponsoring these experiments!

We found that especially small and medium enterprises in digital manufacturing would strongly benefit from technical computing in HPC centers and in the cloud. By gaining access on demand from their desktop workstations to additional compute resources, their major benefits are: the agility gained by shortening product design cycles through shorter simulation times; the superior quality achieved by simulating more sophisticated geometries and physics and by running many more iterations to look for the best product design; and the cost benefit by only paying for what is really used. These are benefits that increase a company's innovation and competitiveness.

Tangible benefits like these make technical computing - and more specifically technical computing as a service in the cloud - very attractive. But how far away are we from an ideal cloud model for engineers and scientists? In the beginning, we didn't know. We were just facing challenges like security, privacy, and trust; conservative software licensing models; slow data transfer; uncertain cost & ROI; availability of best suited resources; and lack of standardization, transparency, and cloud expertise. However, in the course of this experiment, as we followed each of the 192 teams closely and monitored their challenges and progress, we've got an excellent insight into these roadblocks, how our teams have tackled them, and how we are now able to reduce or even fully resolve them.

For this case study from Team 192 two COMSOL applications were used; one 2D model and one 3D model of an industrial fragrance extraction boiler. Both models use specific modeling for mass and heat transfer of fluid flows and immobile solids, built from the COMSOL Multiphysics® Heat Transfer Module.

We want to thank the team members for their continuous commitment and voluntary contribution to this experiment, and thus to our technical computing community. And we want to thank our main Compendium sponsors **Hewlett Packard Enterprise** and **INTEL** for generously supporting these 192 UberCloud experiments.

Now, enjoy reading!

Stephan Savarese*, Wolfgang Gentzsch**, Burak Yenier**

*) ForCES.Paris, **) UberCloud Inc.

***) UberCloud is the online community and marketplace where engineers and scientists discover, try, and buy Computing Power as a Service, on demand. Engineers and scientists can explore and discuss how to use this computing power to solve their demanding problems, and to identify the roadblocks and solutions, with a crowd-sourcing approach, jointly with our engineering and scientific community. Learn more about the UberCloud at: http://www.TheUberCloud.com.*

Team 192

Thermal Modelling of a Fragrance Extraction Reactor in the Cloud with COMSOL Multiphysics

"The use of COMSOL Multiphysics packaged in the UberCloud software container together with the HPC cloud services from CPU 24/7 provides many advantages for the CAE engineer."

MEET THE TEAM

End user – Stephan Savarese, Multiphysics Consultant and Founder at ForCES, Paris, France
Team Expert – Pär Persson Mattsson, Technical Support Engineer and HPC Consultant at Comsol Multiphysics GmbH, Germany
Software Provider – Winfried Geis, Branch Manager at Comsol Multiphysics GmbH, Germany
Resource Provider – Thomas Gropp, Engineer IT-Systems, and Christian Unger, Project Manager Resource Area, CPU 24/7 GmbH.

USE CASE

In this test project for High Performance Computing (HPC) in the Cloud, we wanted to find out how the cloud can help in speeding up and enabling high performance FEM simulations with COMSOL Multiphysics® and COMSOL Server™. The aim of the project was to find out how HPC cloud providers can augment the internal on-premise hardware to allow for more detailed and faster simulations.

COMSOL Multiphysics® is a general-purpose software platform, based on advanced numerical methods, for modeling and simulating physics based problems. COMSOL Multiphysics®, with its multiphysics capabilities, is especially suited for coupled and multiphysics simulations, making the description of real-world multiphysics phenomena and systems possible.

COMSOL Server™ has been created specifically for running and distributing applications built with the Application Builder. It allows you to spread the advantages of simulation throughout your organization and networks. It provides the platform for deploying applications created by simulation experts to your design teams, manufacturing departments, test laboratories, and customers and clients throughout the world. Your colleagues can access and run your apps on COMSOL Server™ through web browsers or a desktop-installed client. The COMSOL Server™ web interface allows you and your colleagues to manage access to the variety of apps you have created, as well as to manage hardware settings and preferences for running the apps.

For this project two COMSOL applications were used: one 2D model and one 3D model of an industrial fragrance extraction boiler. Both models use specific modeling for mass and heat transfer of fluid flows and immobile solids, built from the COMSOL Multiphysics Heat Transfer Module.

These two models were chosen since they represent two frequent options for thermal and fluid flows models. The 2D model enables exploring a wide range of operating condition, while the 3D model is suitable for detailed analysis and optimization. Only one form of parallelization of multiphysics simulations has been tested: shared-memory parallelism (SMP).

CHALLENGES

Both of the models used in this project bring with them their own challenges:

- In the case of the 2D model, phase change has been added to allow for water vaporization. This slows down the computation so much that the simulation takes days on a powerful engineering computing laptop or desktop PC.
- For the 3D model with a large geometry, a large amount of memory is needed to be able to compute the model at all. Many users in small or medium companies do not have the hardware needed on premise, so the cloud provides an ideal hardware extension to handle these types of models sporadically.

PROCESS AND BENCHMARK RESULTS

Computations were performed on cloud resources at CPU 24/7, leading provider of CAE as a Service solutions for all application areas of industrial and academic/university research and development. Headquartered in Potsdam/Germany, CPU 24/7 develops and operates on-demand services for HPC that are based on latest industry standards for hardware, software, and applications. All computations were performed on a single node equipped with dual socket Intel® Xeon® E5-2690 v3 and 256 GB of RAM, giving a total count of 24 cores. This hardware setup was chosen because it is equivalent to the latest Intel desktop workstations suitable for engineering computations. The hardware (bare-metal, non-shared infrastructure) was supplied by CPU 24/7, and COMSOL Multiphysics® was pre-installed on UberCloud's application software container.

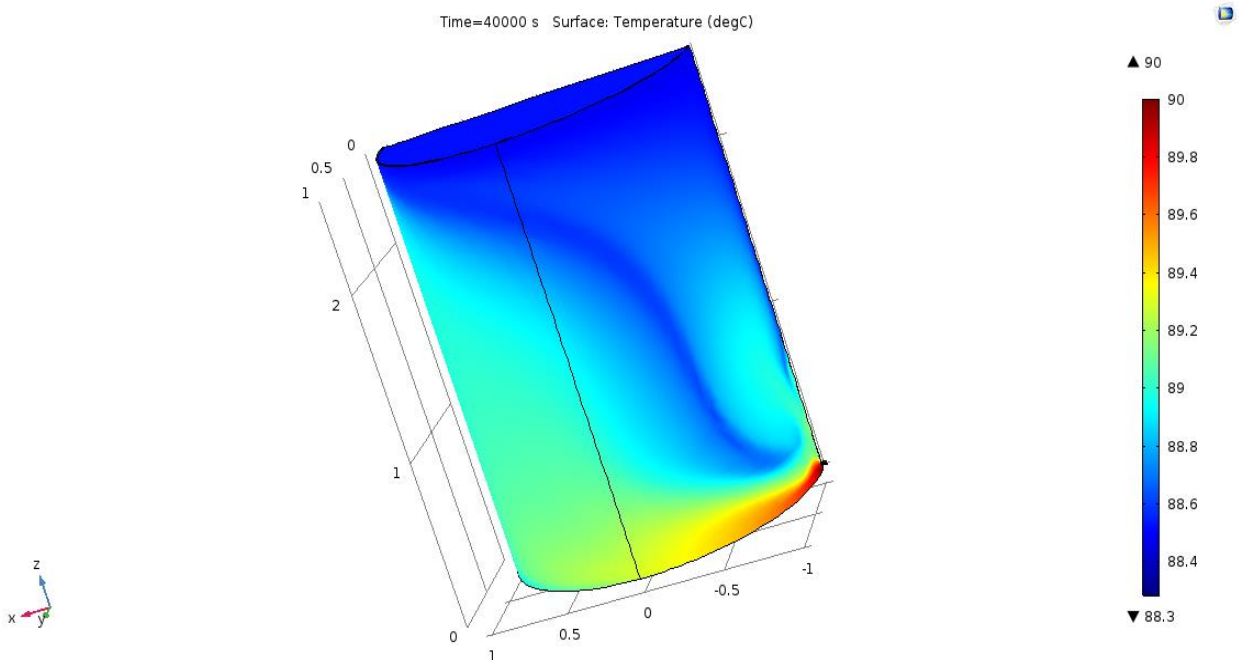

Figure 1 - The heating/cooling sleeve around the reactor is thin. The image shows the surface temperature (in degrees Celsius) of the fluid at the end of the heating phase of the thermal cycle (scale colormap). The swirling flow from the bottom right inlet to the upper left outlet is clearly visible.

Since the COMSOL Floating Network License (FNL) and the COMSOL Server™ License (CSL) allow for remote and cloud computing out of the box, we only needed to use the built-in COMSOL Multiphysics® functionality for starting jobs on remote clouds and clusters, and forwarding access to the on-premise license manager. Once the functionality is configured, any model can be sent to the cloud cluster in a matter of seconds.

The simulations were performed both in the COMSOL Multiphysics environment and on the COMSOL Server.

The remote COMSOL Multiphysics® cloud environment proved to be very responsive and the graphics quality on a large screen was excellent, after setting the proper parameter in the network connection software. This enabled handling the large 3D model without any clumsy delays between mouse operations and GUI response. Furthermore, operations such as meshing and post-processing on a large model took only a few seconds. This pushes the computational modelling limits in terms of precision and accuracy by an order of magnitude compared to regularly available hardware.

On the other hand, the Application Builder is not available from within the Linux container, so the COMSOL Apps need to be built on the local desktop. This is not a problem because building and testing the app in the Application Builder requires less memory and computing power than meshing, solving or post-processing the model. Furthermore, the application can be easily uploaded to the COMSOL Server™ and tested there in the final stages of the building/testing cycle.

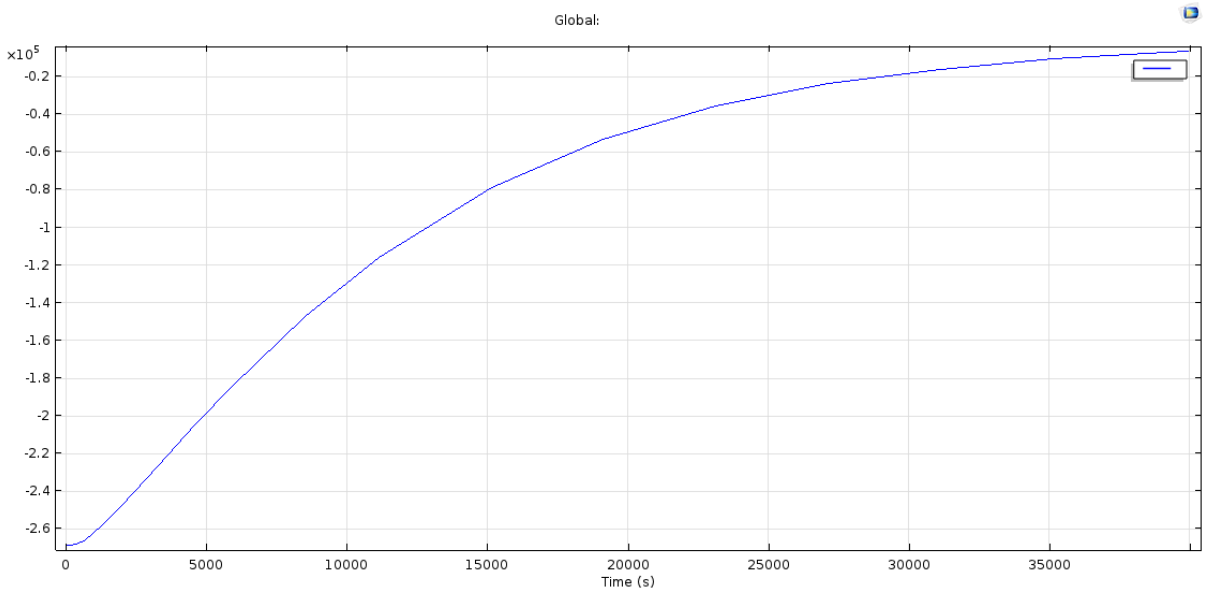

Figure 2 – The heating phase of the cycle is simulated in order to predict the thermal dynamics of the sleeve/reactor assembly. The curve shows the resulting power input (in Watts: note the 1e5 scale, so the numbers actually show negative power input in units of 100 kW) computed from the controlled temperature at the inlet and the computed water temperature at the outlet, thereby yielding the power requirement for the heating boiler.

BENEFITS

For the end-user, the use of COMSOL Multiphysics® from the UberCloud container together with the HPC cloud services from CPU 24/7 brings with it many advantages. A few of them are:

- Increased number of cores and memory channels yield higher throughput for time critical projects.

- The increased amount of memory and the faster memory access obtained from an increased number of cores allows us to compute more realistic and detailed models, which might be impossible to compute on local hardware.
- One can have fast access to a powerful workstation in the cloud, thanks to the fast and competent support from CPU 24/7. Since COMSOL Multiphysics® has been pre-installed in an UberCloud software container, and access to the CPU 24/7 cloud resource was enabled both via remote desktop solutions and SSH, there was no reduction in usability compared to an on-premise workstation.
- The easy access to the cloud through the COMSOL Multiphysics® GUI, and the possibility to forward your license makes it easy to extend your on-premise hardware when needed.

CONCLUSIONS

- It has been shown that the CPU 24/7 HPC bare-metal cloud solution is a beneficial solution for COMSOL users who want to obtain higher throughput and more realistic results in their simulations.
- Using cloud computing removes the need for investment in in-house powerful workstations or servers which are not useful year round. Furthermore, next computing campaigns will benefit from updated hardware and software, since CPU 24/7 offers permanently available and tailored HPC bare-bone cloud solutions.
- Once validated, the containerized environments provided by Uber Cloud were completely set up by the UberCloud team, requiring no end user intervention, except for a few remote computing settings to adapt the screen resolution to the COMSOL GUI size.

Case Study Author: Stephan Savarese, Multiphysics Consultant and Founder at ForCES

Thank you for your interest in the free and voluntary UberCloud Experiment.

If you, as an end-user, would like to participate in this Experiment to explore hands-on the end-to-end process of on-demand Technical Computing as a Service, in the Cloud, for your business then please register at: http://www.theubercloud.com/hpc-experiment/

If you, as a service provider, are interested in promoting your services on the UberCloud Marketplace then please send us a message at https://www.theubercloud.com/help/

1st Compendium of case studies, 2013: https://www.theubercloud.com/ubercloud-compendium-2013/
2nd Compendium of case studies 2014: https://www.theubercloud.com/ubercloud-compendium-2014/
3rd Compendium of case studies 2015: https://www.theubercloud.com/ubercloud-compendium-2015/

HPCwire Readers Choice Award 2013: http://www.hpcwire.com/off-the-wire/ubercloud-receives-top-honors-2013-hpcwire-readers-choice-awards/
HPCwire Readers Choice Award 2014: https://www.theubercloud.com/ubercloud-receives-top-honors-2014-hpcwire-readers-choice-award/

In any case, if you wish to be informed about the latest developments in technical computing in the cloud, then please register at http://www.theubercloud.com/. It's free.