HPC User Forum

April 1-3, 2019 – Santa Fe, New Mexico

Personalized Healthcare with High Performance Computing in the Cloud

“HPC for Doctors”

Wolfgang Gentzsch

The UberCloud

Big Thanks to Hyperion, HPCwire, HPE, Intel,

And to the HPC User Forum Steering Committee for these Awards

HPC as a Service – **For the Masses**

The Partners: Advania / HPE / Intel / Dassault / UberCloud

- **Advania**'s HPC as a Service hardware configuration
- Built upon 100 **HPE** ProLiant (and recently Apollo) servers
- Each with 2 **Intel** Broadwell E5-2683 v4 with Intel OmniPath
- **Dassault Systèmes** SIMULIA Abaqus for structure and advanced electro-physiological interaction
- **UberCloud** HPC containers hosting application workflow
- **Users**: Proof of Concepts with Stanford University Biomechanical Lab & NIMHANS National Institute of Mental Health in Bangalore

HPC as a Service

Core Technology = HPC Containers

- Based on Docker (2013), **enhanced** for engineering & scientific app software
- Application software like Abaqus is **pre-installed**, configured, tested by UberCloud and Stanford
- Includes **all tools** an engineer needs such as MPI and remote visualization
- Running on-prem, and in hybrid and public clouds

Last Year in Tucson, AZ: The Living Heart Project

Studying Drug-induced **Arrhythmias** of a Human Heart with Abaqus in the Cloud

Stanford University

SIMULIA

advania data centres

Uber Cloud

intel

Hewlett Packard Enterprise

HPCaaS Environment and Simulations

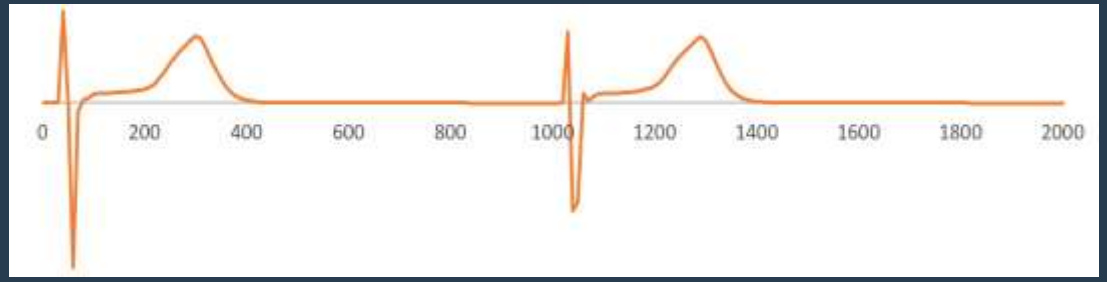
Advania / HPE / Intel / Dassault / UberCloud

Goal: create FEA model and simulations to ENABLE DOCTORS to study drug-induced arrhythmias of a patient's heart, to allow for ambulant treatment

- Hundreds of cloud HPC hours on different Advania configurations
- LHP model scales well up to 240 compute cores
- 42 simulations each 40 hours on 5-node (160-core) subsystem
- Study: identifying drugs causing arrhythmias
- Applying drugs by blocking different ionic currents in cellular model, replicating what has been observed before in cellular experiments
- For each case, we let the heart beat naturally and see if the arrhythmia is developing

Simulation Results

Electrocardiogram (ECG) without and with the drug Sotalol

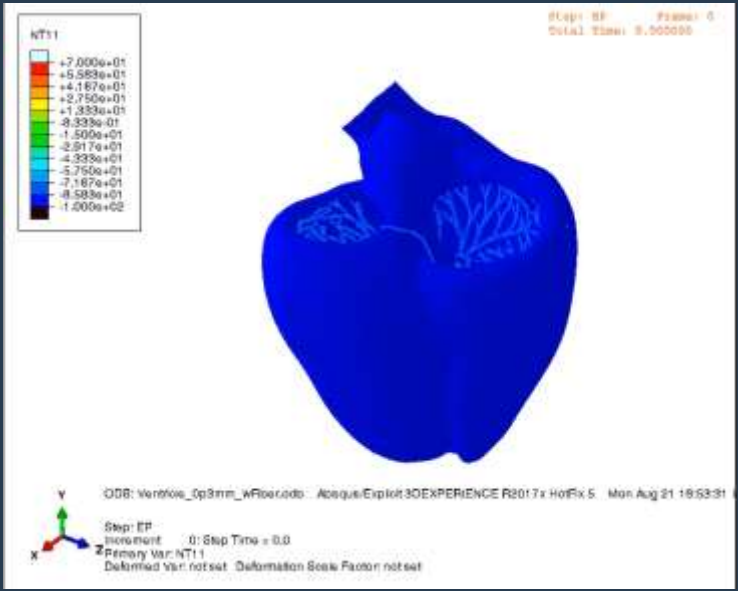


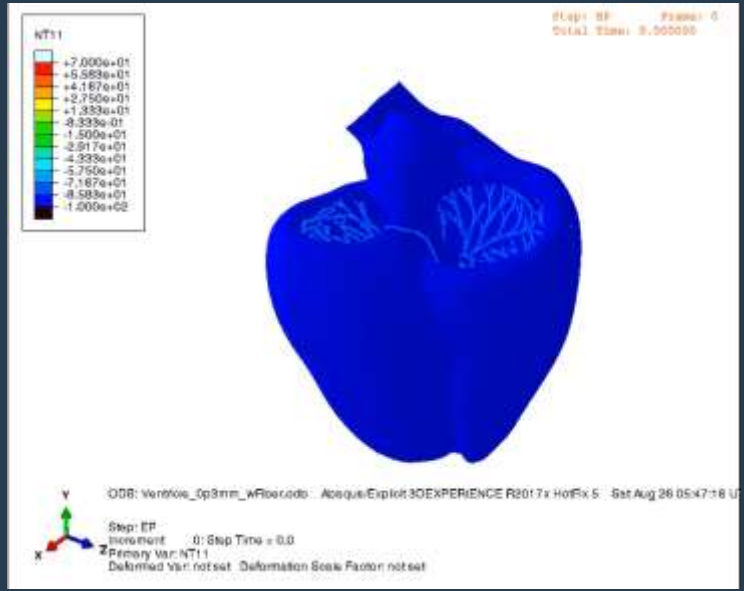
ECG tracing for healthy, baseline case

Arrhythmic development after applying the drug Sotalol.

Note: These are simulation results !

Videos of the healthy case versus the drug-induced case



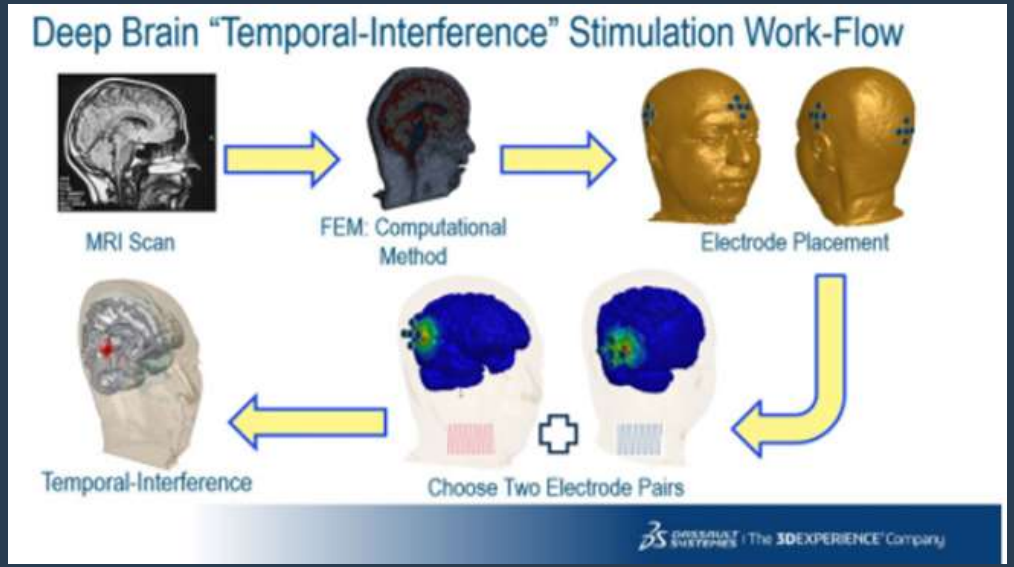


Application of the drug Quinidine (right) where we observe arrhythmia

The Living Brain Project

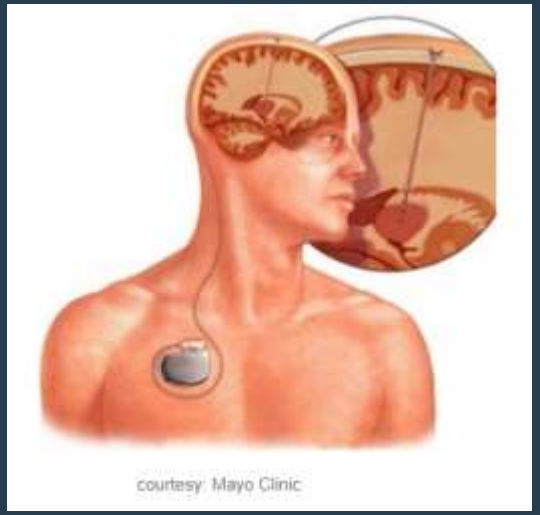
HPC Cloud Simulation of Neuromodulation in Schizophrenia

UberCloud Experiment #200



The workflow for the Virtual Deep Brain Stimulation on a human head model

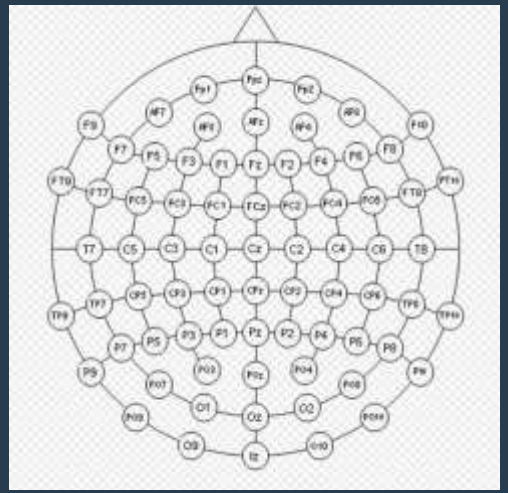
Neuromodulation in Schizophrenia



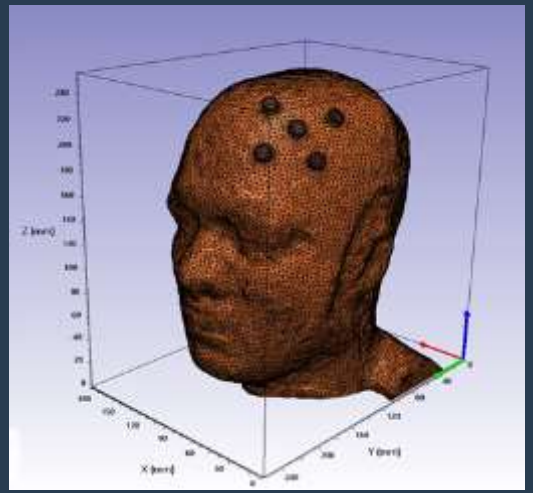
invasive surgeries: drilling small holes in the skull; electrodes are inserted to the dysfunctional regions of the brain to stimulate the region locally

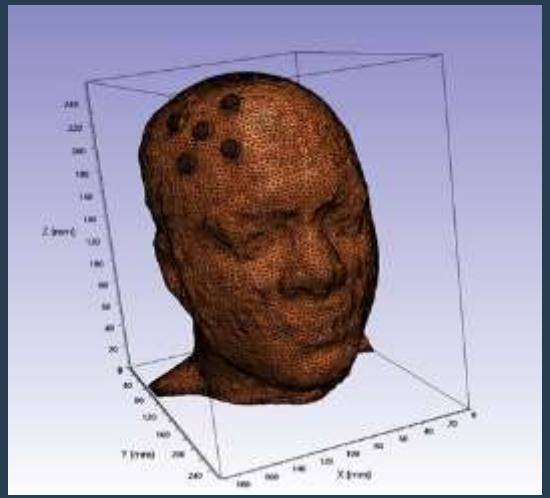
Illustration of non-invasive transcranial Direct Current stimulation device

Electrode Placement



10-10 Electrode system

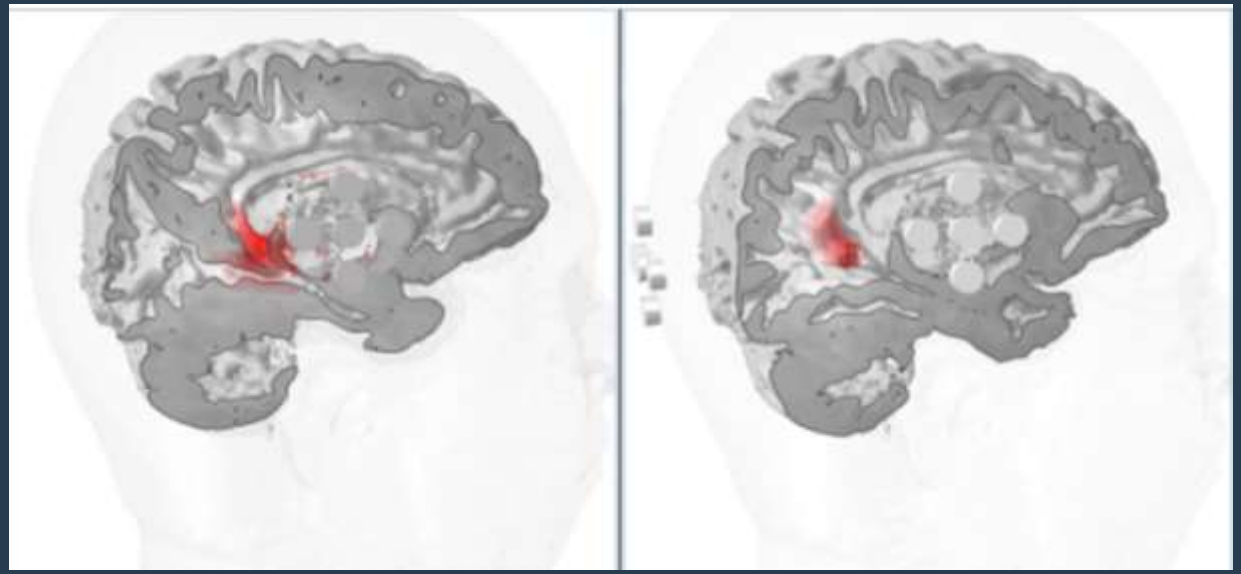




Different electrode placements on Subject’s mesh (ScanIP)

HPC Cloud Simulation of Neuromodulation in Schizophrenia

UberCloud Experiment #200



Sensitivity of the temporal-interference region deep inside the brain based on electrode placement on the scalp

HPCaaS Environment and Simulations

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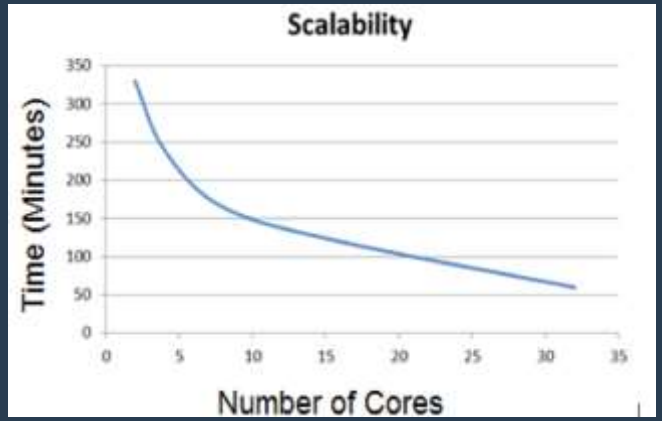
Goal: create FEA model and simulations to ENABLE DOCTORS to study optimal placement of electrodes, to allow for ambulant treatment

- 26 Abaqus jobs 1.8M finite elements each representing a different electrode config.
- 1 job, 16-core, on-prem = 75 min;
  Cloud, 24-core = 28 min => Factor 2.6
- But: 26 independent simulations in parallel, speedup of 26: 33 hours => 28 minutes = speed-up factor of 70
- **T**he patient can wait for his results => **ambulant treatment**



Next step: Apply Deep Learning

First Discovery: Deep Learning for Fluid Flow Prediction in the Cloud

- Apply an ANN to CFD to significantly decrease time-to-solution
- While preserving much of the accuracy of a traditional CFD solver
- Large number of simulation samples and let ANN learn dependencies between simulated design & the flow field around it
- OpenFOAM & TensorFlow in UberCloud HPC container
- 1,000 and 70,000 simulations in Cloud, supported by Renumics and KIT
- Divergence accuracy: 0.94 for 1,000 samples to 0.98 for 70,000 samples

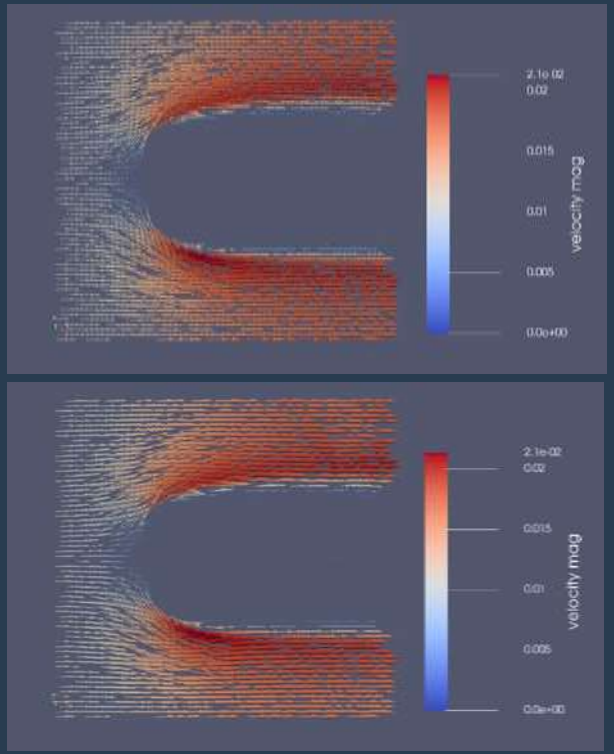
Training Results

- Performance for generating the flow field data set and Tensorflow training

Setup	2-D external flow	3-D internal flow
Time for 10.000 simulations	13.2 h	152.5 h
Time for training	23.7 h	48.5 h

- Neural network prediction of flow field

Setup	2-D external flow	3-D internal flow
Time for CFD solver	4.7 s	55.0 s
Time of neural network prediction	3 ms	120 ms
Speedup factor with deep leaning	**1566**	**458**



Key Take-Aways

- HPC as a Service can assist doctors in personalizing healthcare by providing patient information with higher accuracy in shorter time at reduced cost
- With increasing number of patients treatment the “intelligence” (and prediction accuracy) of Abaqus/TensorFlow container increases
- HPC Containers give us a way to solve software management problems without performance issues
- And, they are able to manage and run most complex engineering workflows
- And, they provide SaaS-like user experience + desktop level ease of use

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Thank You

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Arrhythmia affects millions of people

- In Europe and North America, atrial fibrillation affects about 2% to 3% of the population (2014)
- Atrial fibrillation and atrial flutter resulted in 112,000 deaths in 2013, up from 29,000 in 1990
- Sudden cardiac death is the cause of about half of deaths due to cardiovascular disease or about 15% of all deaths globally
- About 80% of sudden cardiac death is the result of ventricular arrhythmias
- Arrhythmias may occur at any age but are more common among older people

Multiscale model of cardiac electrophysiology

- Bi-ventricular anatomy based on healthy human
- Finite element model with 7,500,000 nodes
- 250,000,000 internal variables, updated/stored within each sim step
- 1,000,000 time steps
- State of the art representation of cellular dynamics
- 3 different cell types in the ventricular wall
- High fidelity model of the Purkinje network