Supercomputer applications in Biomedical engineering – from simulation to PoC and production

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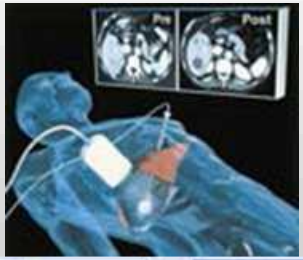
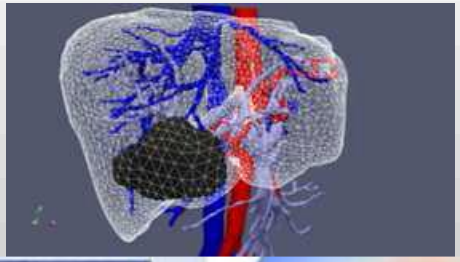
AMET Ltd.

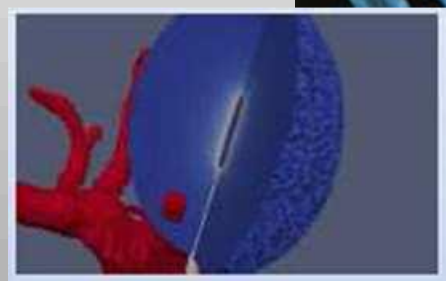
- Established in 1995 AMET Ltd. is a company dedicated to development, modern manufacturing and distribution of electronic medical equipment and modules.
- The company is a reliable and desired partner in both the Bulgarian and the foreign market.
- The partnership between IICT-BAS and AMET Ltd. is directly based on the development of computer models.and their efficient implementation on HPC systems.
- The products, developed or/and upgraded within the several joint projects frame include:
  - Smart electrosurgical instruments: Together with imaging techniques for diagnosis, an active electrode is placed in the center of the tumor and, using controlled high-frequency current and saline enhancement, thermal destraction of the target volume is achieved.
  - Physiotherapy equipment: A portable device for removing ticks and leeches on people or pets via high-frequency electrical impulses, without touching the body of the parasite.
- AMET Ltd. is an associated industrial partner at the Center of Excellence in Informatics and Information and Communication Technologies, financed under contract BG05M2OP001-1.001-0003 by Operational Program “Science and Education for Smart Growth”2014-2020.
- AMET Ltd. was a partner in the organization of the “13th International Conference on Large-Scale Scientific Computations”, June 7-11, 2021.

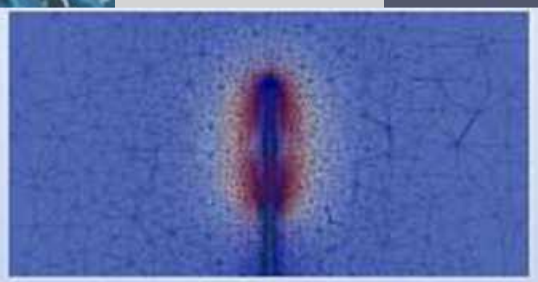
Radio-frequency Liver Ablation

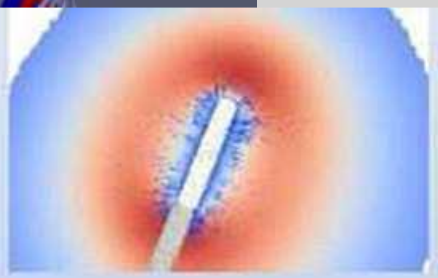
- Radio-frequency ablation (RFA) destroys the undesired tumor tissue heating as a result of a radio-frequency alternating current flow, delivered by a needle-like RFA probe.
- To establish the model, the geometry of the volume of interest as well as the microstructure of the corresponding body tissues are extracted from a 3D high-resolution digital image.
- For the discretization of the corresponding system of Partial Differential Equations that describes the ablation processes, a Finite Element Method on unstructured tetrahedral mesh with an adaptive time step is applied.
- The derived computer model possesses up to $O(10^9)$ unknowns with respect to the space variables and $O(10^4)$ time steps. For numerically solving problems of such a computational complexity it is a necessity to incorporate an HPC system.







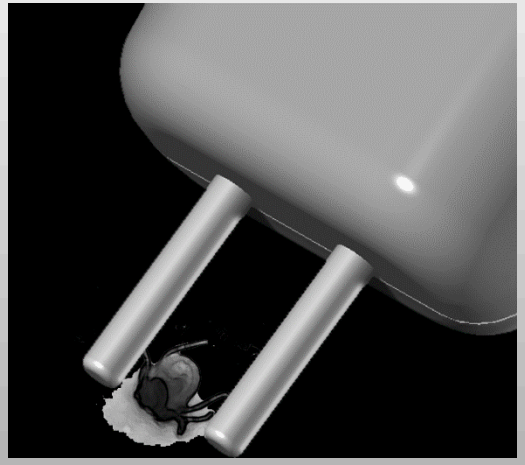




Contact-free tick removal

- The portable device for removing ticks, leeches and other blood-sucking ectoparasites on people or pets uses radio-frequency electrical impulses.
- It is essential that the physiotherapeutic procedure is performed without any contact between the device and the parasite body. Thus the danger of blood infection due to liquids, excreted by the parasite during the removal process, is avoided.
- A subject of Computer Modeling is the analysis on the temperature field within the impact region.
- The process is described via a system of Partial Differential Equations.
- For the PDE discretization, a Finite Element Method on unstructured tetrahedral mesh is applied.

- The computational region possesses a complicated, multi-layer geometry, including a thin film with respect to the applied gel and the skin layers.
- The computational complexity of the problem is determined by both the strong mesh and coefficient anisotropy.

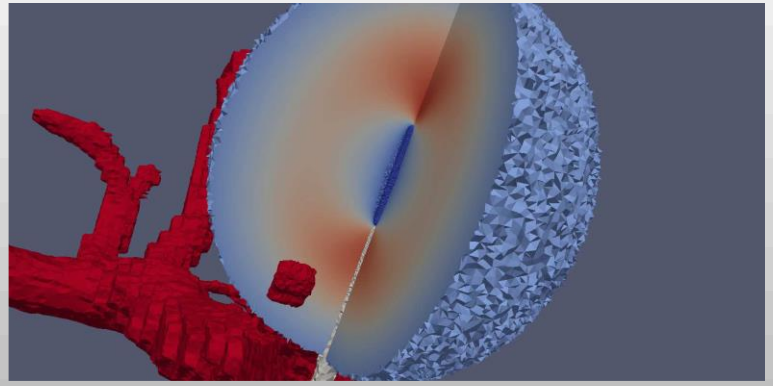


Mathematical and Computer Modeling

The mathematical model, together with the computer one include:

- Discretization in space of the Partial Differential Equations. For this purpose, a Finite Element Method on unstructured tetrahedral meshes is applied.
- Discretization in time of the Partial Differential Equations. For the purpose, specialized algorithms with an adaptive time-step have been developed.
- Generation of three-dimensional tetrahedral meshes, adaptively refined within the regions of active interactions.
- Identification and verification of the model parameters. For the purpose, least-squares-type optimization is applied.

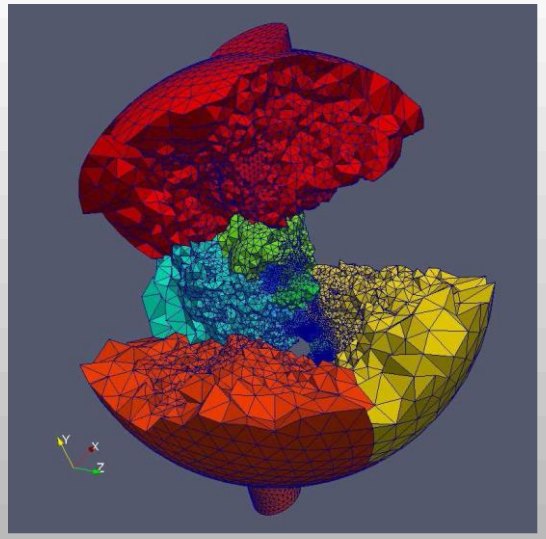
- Iterative methods with optimal computational complexity for solving large scale (up to 10^8-10^9 unknowns) linear systems with sparse matrices.
- Visualization of the results, including isolines on electric and temperature fields, and extraction of integral results from large data arrays.



Parallel Implementation

The parallel realization of the developed computer models involves integration of open-access parallel software packages, such as:

- **Netgen**: High-performance software package for a FEM realization. In the developed software solutions, the module for 3D mesh generation has been used. The parallel kernel is written in C++'
- **ParMETIS**: Parallel partitioning of unstructured graphs and numeration reordering with the aim of minimizing the filling of sparse matrices during the process of consecutive elimination. In the developed software solutions, the package is used for subdividing the computational region into sub-regions.
- **Hypre**: A software library for a scalable parallel realization of the preconditioned conjugate gradient method. It is developed and supported by the Lawrence Livermore National Laboratory.
- **BoomerAMG**: A part of Hypre, devoted to the realization of an optimal algebraic multigrid preconditioner.
- **ParaView**: A parallel platform for analysis and visualization of high-dimensional data.



A Parallel Computational Model

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- The parallel realization is built upon a computational model with distributed memory. This allows for solving large-scale problems with *O(10^9)* DoFs.
- The contemporary supercomputers, including the supercomputer system Avitohol at IICT-BAS, are with distributed memory.
- Communications are realized with the help of MPI.
- The realized computer models are strongly coupled, which determines the key role of the communications.
- It is shown that for the considered class of problems 1D and/or 2D domain decomposition (partitioning) leads to highly restricted parallelism. For example, in the case of 1D partitioning, the parallel efficiency E_P may drop down to under 1%.
- Here, it is important to point out that for engineering applications, which involve solving linear systems with sparse matrices, the supercomputer performance is substantially lower than the peak one.

This, of course, does not mean that such problems should not be considered!

- <u>Parameters for the considered problems</u>:

  - number of unknowns in the coupled systems: up to 1 117 913 088
  - number of processors or CPU cores: up to 1 024
  - maximal parallel efficiency achieved: above 100%

Performance and Efficiency of the Supercomputers

LINPACK: A software library for performing numerical linear algebra on digital computers. There is a benchmark test for determining TOP500 – the ranking of the top 500 supercomputers in the world. The criterion is based on the time for solving a linear system with a dense matrix.

Unlike measuring the peak performance Rpeak, the above test gives rise to an easy comparable evaluation of the achieved performance Rmax with respect to the test.

For the top 10 supercomputers in TOP500 the following averaged efficiency has been documented:

June 2019: Rmax/Rpeak = 71%

June 2020: Rmax/Rpeak = 73%

Avitohol: Rmax/Rpeak = 64%.

We can draw the conclusion, that the LINPACK efficiencies are comparable.

HPCG: An alternative benchmark test for performance evaluation, based on iterative solving of linear systems with sparse matrices, applying the conjugate gradient method. In this way, the HPCG performance values are computed and the corresponding averaged efficiency is:

June 2019: HPCG/Rpeak = 2.59%

June 2020: HPCG/Rpeak = 2.23%

It is not surprising that the HPCG efficiency is substantially smaller. On the other hand, it is important to note that this efficiency is more representative.

The impact of the model complexity on the numerical results

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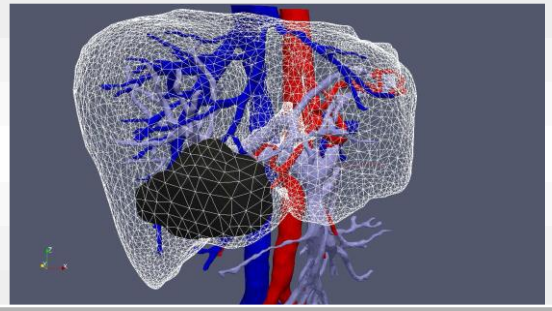
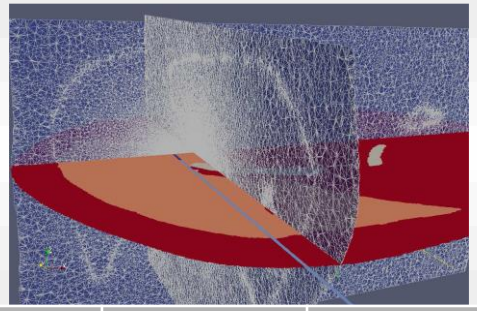
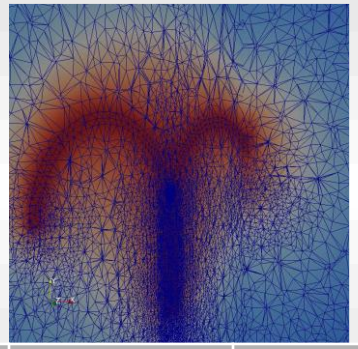
- The process of tumor ablation is substantially three-dimensional and time-dependent (nonstationary).
- The model incorporates an electric field, a mass and heat transfer, a flow in porous media, cells destruction, etc.
- The computational region is strongly inhomogeneous, with gives rise to the usage of a strongly unstructured triangulation.



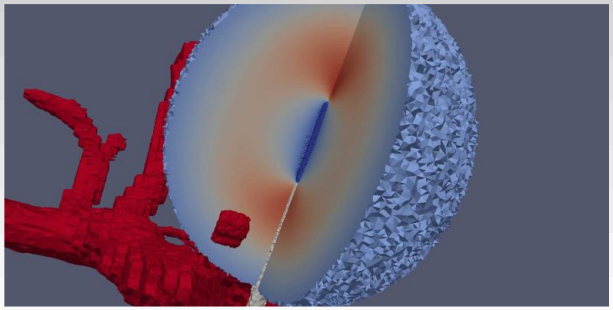


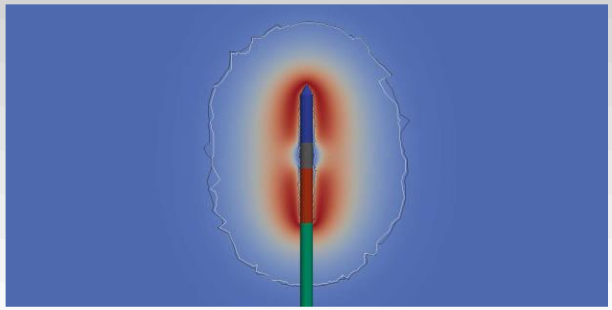


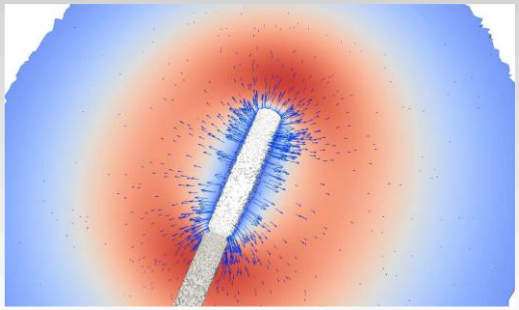
Model	V_1[cm^3]	Difference	$V_{4.6}$[cm^3]	Difference
Does not take into account the blood circulation	20.7		14.0	
Takes into account the blood circulation in the portal vein	10.8	191%	6.7	209%
Takes into account the portal vein and the capillary network	7.8	265%	5.3	284%

- In the table by V_1 and $V_{4.6}$ are denoted the volumes of effective ablation, for which the tumor cells are destroyed with probability 66% and 99%, respectively.

Full parallel scalability







N	p	Δt[s]	N_{it}	T[s]
2 183 424	128	5	642	1 723
17 467 392	1 024	1.25	1 610	6 170

- A 6-minutes process of radio-frequency ablation with a bipolar probe is simulated.
- For the refined model 8 times more processors are used with 8 times more degrees of freedom N at each time step.
- Meanwhile, 4 times more time steps are needed but the parallel execution time is just 3.58 times higher.
- Therefore, for the full parallel efficiency of the model we derive E_{total} = 111%.

Opportunities and Challenges

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- The new opportunities and challenges are determined by the evolution of the HPC technologies and the comprehensive tendency for working in a Big Data environment.
- The above determines the key role of the synergy between HPC simulations and AI for Big Data.

Examples:

- In the needle-like probes of the contemporary devices for radio-frequency liver ablation more and more sensors are integrated, which provide continuous information on a number of parameters, related to the ongoing processes, such as temperature and electrical resistance. Meanwhile, the applied imaging diagnostics tools generate huge data sets of medical images. In order to process and/or analyze such big data, specialized algorithms for HPDA/AI are needed to be implemented.
- The constantly growing HPC systems performance allows for the realization of the concept for „Modeling, Simulation, and Optimization“ – the mathematical foundation of the “digital twin” technology.
- The beginning of the realization of those opportunities is laid by our joint work on building an integrated software platform for tuning the parameters, involved in the radio-frequency liver ablation model. The main challenge is the data base processing of the particular patient in real time.