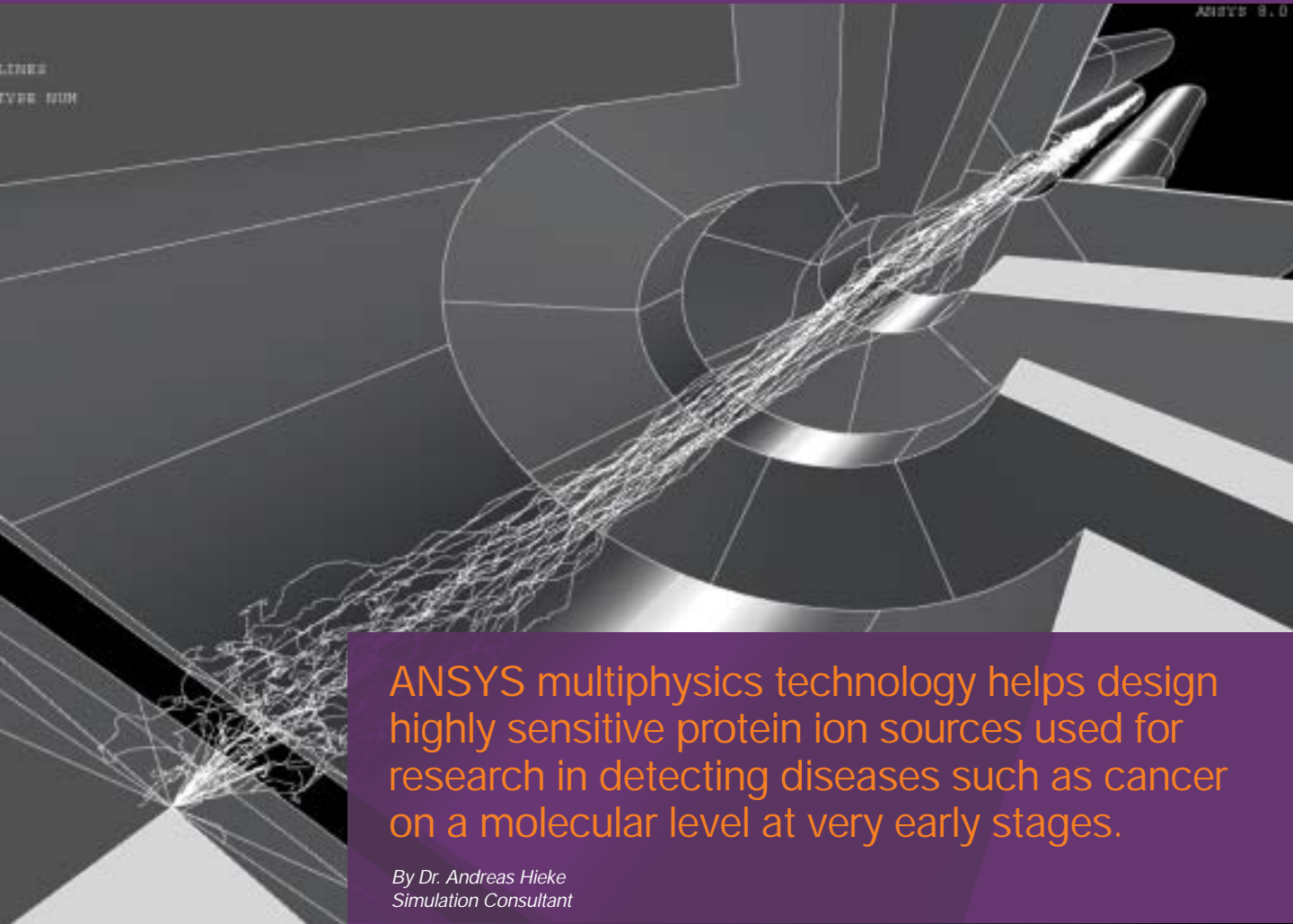


# Ion Dynamics in Electro-Pneumatic Fields: A Key to Modern Biotechnology

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ANSYS multiphysics technology helps design highly sensitive protein ion sources used for research in detecting diseases such as cancer on a molecular level at very early stages.

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The area of protein research known as “proteomics” attempts to identify patterns of proteins (“biomarkers”) that correlate with disease states. The goal is to detect diseases, such as cancer, on a molecular level at very early stages when treatment is far more effective, while causing substantially fewer side effects.

However, biological macromolecules with masses on the order of  $m=10^3$  to  $10^6$ u remained inaccessible for mass analysis until the 1980s due to a lack of suitable soft ionization methods and available instruments for these masses. While instrument performance was gradually improved with the advent of cheap solid-state memory, fast PCs and ultra-high-speed ADCs, it was the invention of a fundamentally new ionization method called MALDI (Matrix Assisted Laser Desorption and Ionization) by Koichi Tanaka et al. in 1987 that opened the door for easy, widespread mass analysis of biomolecules and for which Tanaka received one-quarter of the Nobel Prize in Chemistry in 2002. [1]

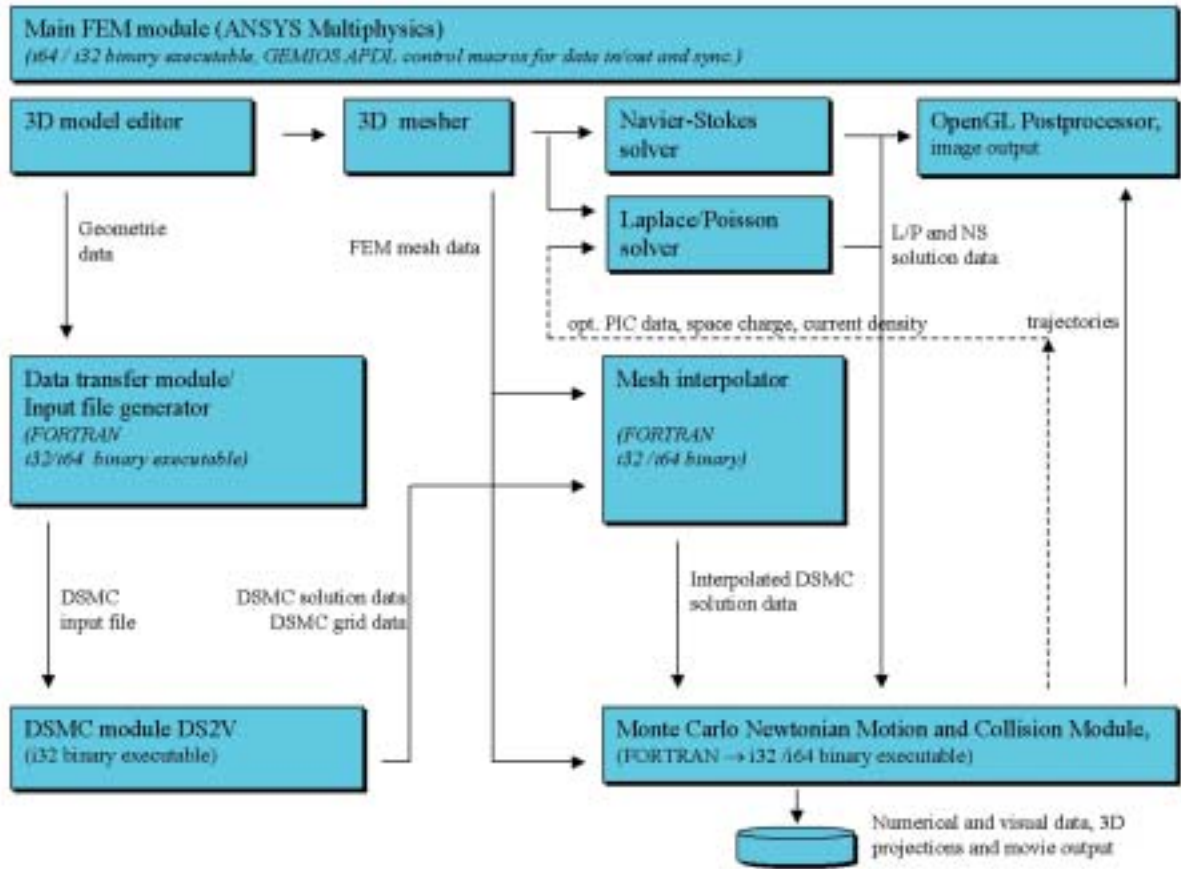


Figure 1. Simplified structure of GEMIOS

One fundamental problem associated with MALDI ion sources is the fact that ejected ions have substantial translational and internal temperatures, which frequently result in molecular fragmentation and decay, thereby limiting the available ion lifetime for analysis.

Experiments carried out in the early 1990s [2] indicated improved ion transmission within gasfilled multipole ion guides due to “collisional cooling.” Repeated collisions of ions with gas molecules reduce the temperature of the ions and also cause the ion beam to collapse axially inside multipole ion guides.

### The Challenge

However, ion optical systems of practical interest operate under conditions and at elevated pressures where electromagnetic forces and molecule-ion scattering effects are equally important, and both gas flow and electromagnetic vector fields vary spatially. Therefore, the understanding and practical design of advanced ion sources for collisionally cooled biomolecules required a novel simulation tool that would allow

the computation of 3-D trajectories and energy exchange of ion beams/clouds under the influence of 3-D time-dependent electromagnetic fields in the presence of 3-D rarefied gas flow fields. While the computation of charged particle trajectories in electromagnetic fields is well known and a number of tools exist, there was no 3-D capable tool that could compute the flow field of rarefied compressible gases AND compute time-dependent electromagnetic fields AND determine the motion and energy exchange of charged particles under the influence of these fields.

The subsequently outlined implementation of such an advanced multi-physics simulation system, henceforth referred to as GEMIOS (Gas and Electromagnetic Ion Optical Simulator), was only possible by utilizing a combination of commercial (ANSYS) as well as special-purpose codes (FORTRAN). The fundamentally novel aspect of GEMIOS is that it combines electromagnetic field solutions and fluid dynamic field solutions obtained within a given domain to compute charged particle trajectories. GEMIOS provides particle energies; collision rates;

translational, thermal and kinetic temperatures; with spatial and temporal resolution. Subsequent research and GEMIOS simulations by the author led to the creation of the new term “electropneumatic ion optics” since the functionality of the considered ion-optical devices is in fact based on the superposition of at least two vector and one scalar field.

Since the development of GEMIOS had to be achieved within a time frame of several months (versus tens of man-years), it was clearly impossible to start at source code level from scratch. The 3-D model generation, meshing and post-processing capabilities required for a large-scale multiphysics system such as GEMIOS exceed the capabilities achievable by an individual and demand the utilization of commercial codes as far as possible.

ANSYS Multiphysics software was the ideal candidate for that role due to its inherent flexibility, complete data access and controllability via APDL (ANSYS Parametric Design Language), as well as

proven meshers and solvers. Thereby, the overall costs for the GEMIOS project have been significantly smaller compared to an entirely new simulation system coded from scratch.

As mentioned, GEMIOS achieves its functionality by utilizing a combination of codes operating on the same input data set (Figure 1):

- a 3-D Monte Carlo-Newtonian Motion and Collision module (MC-NMC), FORTRAN
- the FEM system ANSYS Multiphysics
- a semi-statistical 2-D DSMC (Direct Simulation Monte Carlo) module for rarefied gas flow

ANSYS Multiphysics serves as a fully parameterized 3-D solid modeler and mesher and provides the 3-D Laplace/Poisson solver for the computation of electromagnetic fields. According to the number of electrodes within a model and based on a set of canonical Dirichlet boundary conditions, a data set of static, orthogonal base solution is computed from which any arbitrary static or dynamic field configuration is later obtained by superposition in the MC-NMC. [3]

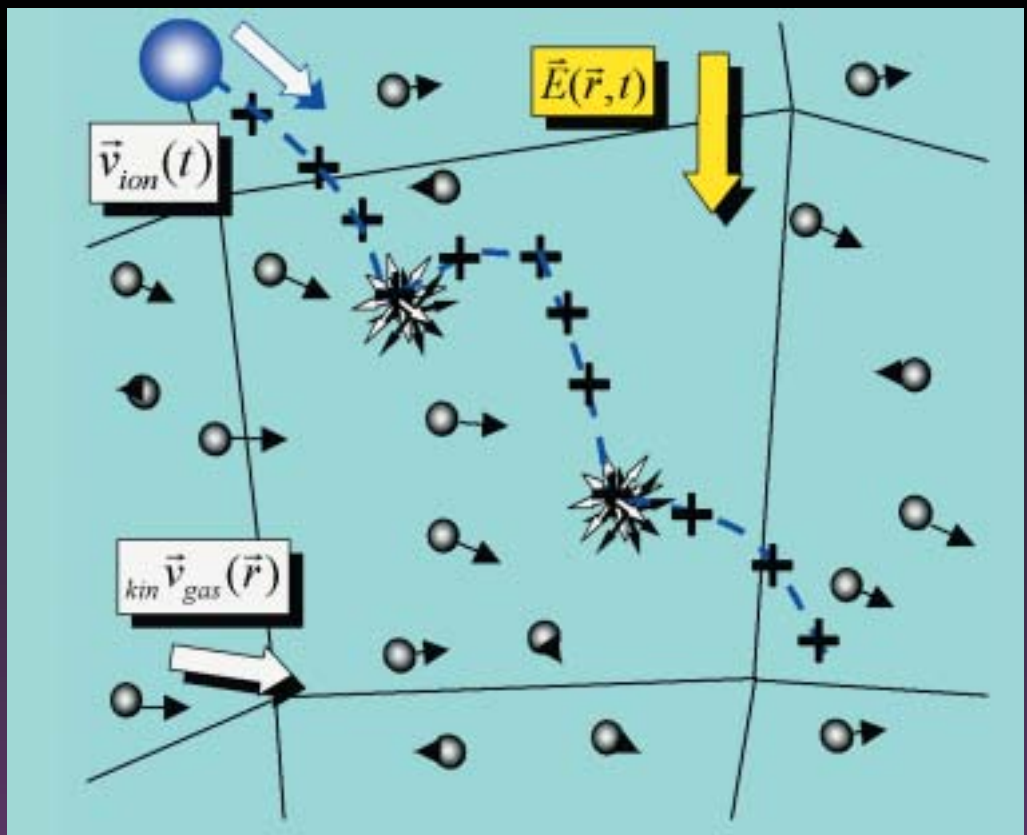


Figure 2. GEMIOS MC-NMC principle: For ions (big sphere) moving through the meshed domain under the influence of a time-dependent electric field at each time step (crosses), a local collision probability is computed. If a collision event occurs (stars), Monte Carlo sampled post-collision velocity vectors are computed.

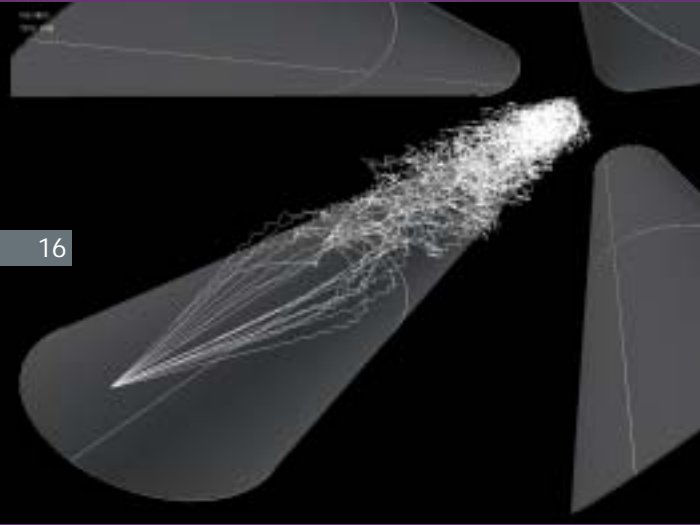


Figure 3. GEMIOS simulation of ion injection into a RF quadrupole:  $m_{ion} = 1000u$ ,  $f = 500\text{kHz}$ ,  $U_{AC} = 500\text{V}$  (field solutions and trajectory visualization via ANSYS)

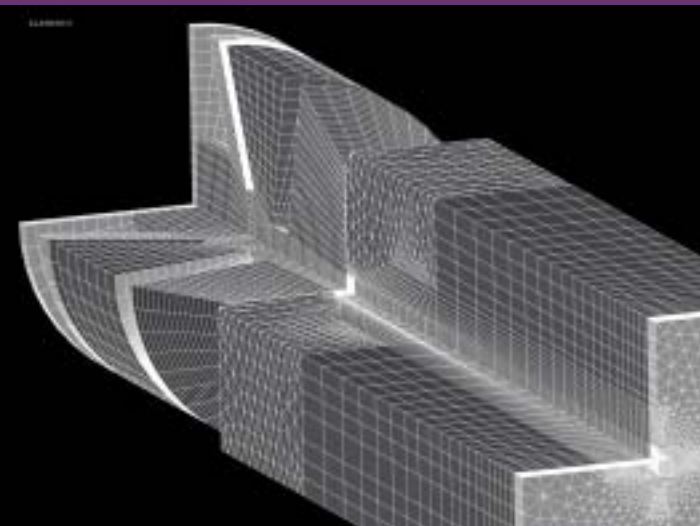


Figure 4. Meshed 3-D model of a quadrupole coupled to an ion generation system; note the great range of used element sizes.

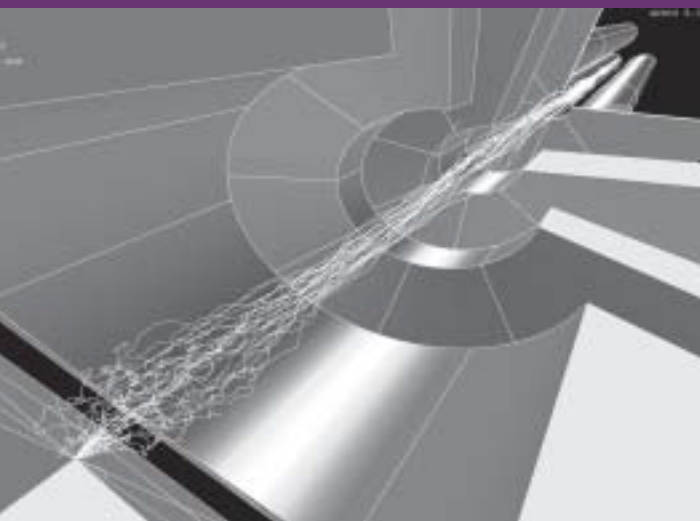


Figure 5. GEMIOS simulation of ion trajectories based on simultaneous consideration of RF electric fields and gas flow fields (field solutions and trajectory visualization via ANSYS)

ANSYS Multiphysics also provides a 3-D Navier-Stokes (NS) solver operating on the same mesh generated for the Laplace/Poisson solution and providing gas pressure, velocity distribution and temperature data of a background gas which is present in the considered ion-optical device. It is particularly advantageous for subsequent computations to obtain electromagnetic and gas flow solutions on the same mesh, although optimal mesh distributions typically differ for both cases.

The FEM NS solver solutions are only valid in regions with a ratio of mean-free path to geometry scale (Knudsen number) on the order of 0.1 or lower, commonly referred to as continuum range. However, the exact Knudsen limit of Navier-Stokes solver is debatable and depends also on the specific case. It is, therefore, of great practical value to compare Navier-Stokes solutions to results obtained by DSMC. Since DSMC is not based on macroscopic properties or derived from macroscopic behavior (as Navier-Stokes is) but rather simulates a gas by actually treating corpuscular collisions of a very large number of virtual super particles in a Monte Carlo algorithm, it is capable of providing unconditionally stable and valid gas flow data at any pressure, Knudsen and Reynolds number. [4]

The 3-D Monte Carlo-Newtonian Motion and Collision module (MC-NMC) is the core component of GEMIOS and computes trajectories and energy exchange of an ion beam/cloud under the influence of provided time-dependent electromagnetic fields in the presence of background gas flow. Monte Carlo simulations of time-dependent properties of ion populations in RF electromagnetic fields necessitate a large number of particles ( $1E3 \dots 1E5$ ) and extended numbers of trajectory integration time steps ( $1E4 \dots 1E7$ ). One additional challenge arising from the use of a FEM system is the computation of particle trajectories in arbitrary meshes [5], which is far more complicated compared to equidistant orthogonal grids used by FDM, commonly found in particle tracing codes. Due to these computational requirements, a separately compiled stand-alone FORTRAN code had to be used for the MC-NMC.

During tracing, and based on local gas density, (MC sampled) temperature, gas flow field velocity, scattering cross-sections, actual ion velocity and current time stepping, a local, time-dependent probability for a collision event is computed. If in fact a collision event occurs, the post-collisional ion velocity is determined based on said local quantities and an additional MC sampling of angular velocity distributions as required for hard sphere models (Figure 2). This procedure replicates aspects of the before-mentioned DSMC approach. Finally, the MC-NMC module extracts time-dependent kinetic, translational

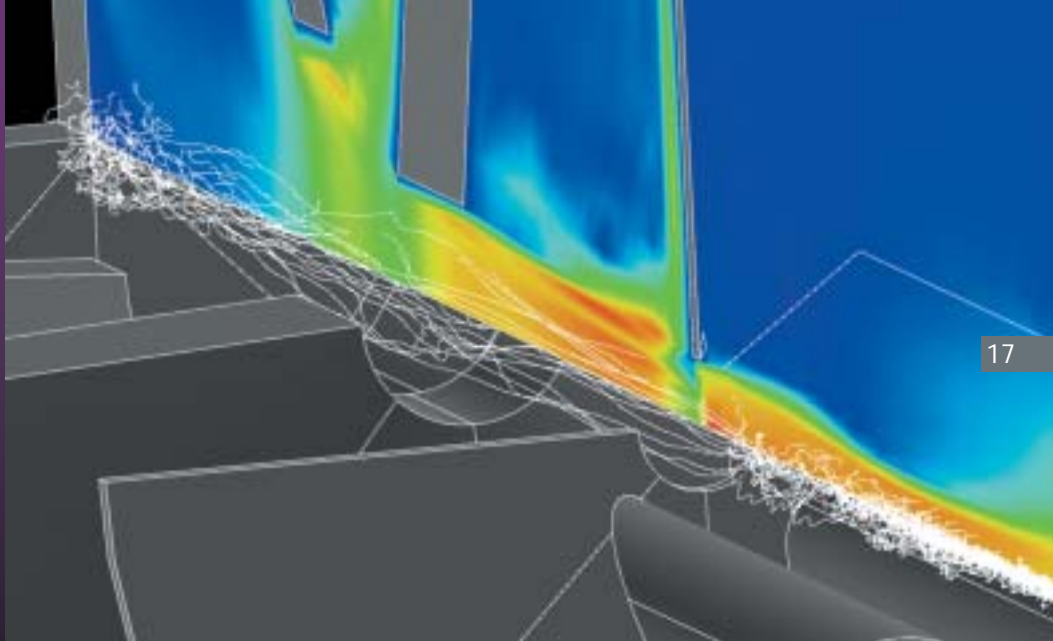


Figure 6. Ion trajectories with superimposed NS solution (contour plot of gas flow velocity)

and thermal energies. It also provides graphical output capabilities (2-D projections) for very rapid animations and/or generation of movies of the computed events. Trajectory data can also be transferred back to ANSYS in order to utilize its post-processor for 3-D OpenGL visualization. [6-10]

## Results

The accuracy of the trajectory integration (without collisions) and field superposition has been verified for a number of cases with known analytical solution of trajectories and fields. The verification of the correct algorithmic approach employed test cases with simple thermal equalization and/or constant gas flow speeds.

GEMIOS continues to provide invaluable insight into the operation of realistic 3-D electro-pneumatic configurations, specifically phenomena such as collisional cooling, heating and focussing of ions (Figure 3 – Figure 5). Movies derived from these simulations have enabled a better understanding of dynamic processes such as RF quadrupole ion injection and associated collisional effects.

Once more, ANSYS proved to be a nearly perfect vehicle in a tricky, highly specialized multi-physics adventure, specifically due to its well documented script-controlled read/write access to all relevant model and solution data. ■

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