

Development of an Advanced Simulation System for the Analysis of Particle Dynamics in LASER based Protein Ion Sources

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ABSTRACT

An advanced multi-physics simulation system henceforth referred to as GEMIOS (Gas and Electromagnetic Ion Optical Simulator) has been implemented which allows the computation of 3D trajectories and energy exchange of ion beams/clouds under the influence of 3D time-dependent external electromagnetic fields in the presence of 3D rarefied gas flow fields and has therewith capabilities beyond existing tools. GEMIOS achieves its unique capabilities by utilizing 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.

1. INTRODUCTION

The goal of clinical proteomics is to identify proteins which may be used as biomarkers and to correlate them with disease states. ProteinChip arrays serve to selectively capture proteins prior to further detailed analysis in specialized mass spectrometers (ProteinChip Readers). A principal and critical step in this process, performed in laser based systems called MALDI (matrix-assisted laser desorption/ionization) /SELDI (surface-enhanced laser desorption/ionization) sources or interfaces, is to generate, cool, and collimate ion beams of said captured proteins to allow injection into mass analyzing devices. Within these interfaces and devices protein ions are subjected to time dependent electromagnetic fields as well as collisions with intentionally introduced background gas molecules in order to reduce the ion temperature. The particle dynamics in such ion sources is extremely complex.

A simulation tool was needed which can provide insight into and a deeper understanding of ion extraction, collisional cooling and guidance processes in the presence of background gases. It also serves to optimize geometric shapes, electric potentials, frequencies, timing, gas flow rates and pressures.

2. METHODS

GEMIOS's capability to provide electromagnetic field solutions and fluid dynamic field solutions is essential to model ion optical systems operating at elevated pressures

where electromagnetic forces and scattering effects are equally important. GEMIOS achieves this by utilizing a combination of codes (Fig.1) operating on the same input data set:

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

ANSYS serves as fully parameterized 3D solid modeler and mesher and provides the 3D 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 (Hieke [1]).

ANSYS also provides a 3D Navier-Stokes 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 DSMC module provides solutions for rarefied gas flow below the continuum range. 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 valid gas flow data at any pressure, Knudsen and Reynolds number (Bird[2]).

The 3D 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 time dependent external electromagnetic fields in the presence of a background gas flow field. While particle tracing is possible in ANSYS using APDL (ANSYS Parametric Design Language) its execution speed is insufficient for Monte Carlo simulations (Hieke [3]). As a result, a compiled stand-alone code had to be used for the MC-NMC.

One of the challenges arising from the use of a FEM system is the computation of particle trajectories in arbitrarily meshes (Kenwright et al. [4]) which is far more complicated compared to equidistant orthogonal grids used by FDM, commonly found in particle tracing codes.

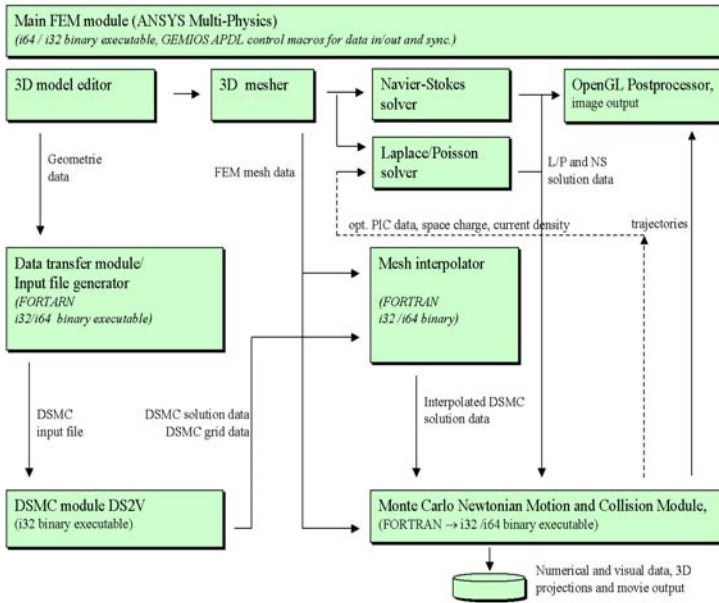


Fig.1: Simplified structure of GEMIOS

First, the MC-NMC reads in files containing information about the structure of the mesh such as node locations, connectivity, element to node correlation, element neighbors, and element center locations. It then builds various cross-reference and lookup tables and employs local search routines to avoid prohibitively expensive brute-force search routines during tracing. Thereby accurate first guess predictions for the element a particle is about to fly in with probabilities on the order of 80 to 90% are achieved.

Second, the MC-NMC reads the orthogonal Laplace base solutions for all nodes and performs a field superposition either globally, prior to the tracing for electrostatic cases, or locally in real time for time-dependent cases. Third, the MC-NMC module optionally reads in gas pressure, velocity and temperature data for element center locations if collisions are computed. In addition, information about particle masses and scattering cross sections must be provided.

The trajectory integration is based on a Runge-Kutta scheme with 2nd order accuracy in time and space with optionally automatic time stepping. Additionally, the MC-NMC employs local interpolation of electromagnetic fields within each element. Details are beyond the scope of this paper and will be reported elsewhere.

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 (Fig. 2). This procedure replicates aspects of the before mentioned DSMC approach. In future, additional collision models as well as rotational and internal degrees of freedom may be implemented. Finally, the MC-NMC module extracts time-

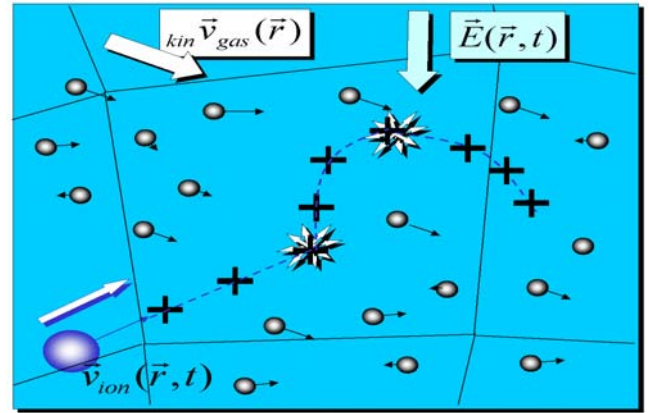


Fig.2: For ions (blue sphere) moving through the meshed domain under the influence of a time- dependent electric field a local collision probability is computed at each time step based on current ion velocity, ion-gas scattering cross section, local gas flow speed, pressure, and Monte Carlo sampled gas temperature. These quantities and the ion mass are also used to determine post-collisional velocity vectors if a collision event occurs (stars).

dependent kinetic, translational, and thermal velocities. It also provides graphical output capabilities (2D projections) for very rapid animations and/or generation of movies of the computed events. Trajectory data can also be transferred to the ANSYS postprocessor for 3D visualization.

3. RESULTS

Trust in such a complex simulation system has to be established gradually by going from simpler to more complex models. 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 including long term dynamic stability in RF quadrupoles. The verification of the correct algorithmic approach of the collision treatment is more difficult. Appropriate test cases involve simple thermal equalization and/or constant gas flow speeds.

The application of electric RF fields in combination with background gas collisions introduces new phenomena such as collisional cooling and heating of ions for which analytical solutions are typically not available (Moore [5]).

Fig. 3 though Fig. 10 show some of such increasingly complex cases computed with GEMIOS ranging from simple ion plume expansion into resting background gas of constant pressure to RF quadrupole confinement and cooling as well as multi-electrode ion source systems.

The computational expense in terms of floating point performance and required memory is substantial. GEMIOS runs on a computer system comprising a dual Itanium2 64bit machine with 12Gbyte RAM, a dual Xeon 32bit machine with 4Gbyte RAM connected via Gigabit Ethernet and an external Arena 8-disk RAID-0 unit for temporary data storage with sustained I/O data rates on the order of 160Mbyte/s.

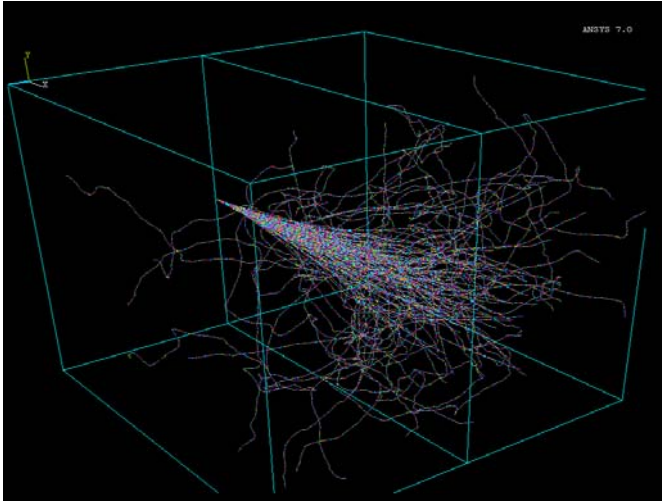


Fig.3: Simple test case: ion beam expanding into resting background gas, no external electromagnetic field, $m_{ion}=1000u$, $d=1nm$, $v_{x0}=1000m/s$, $T_{gas}=300K$, $p_{gas}=0.1Pa$, $v_{gas}=0m/s$

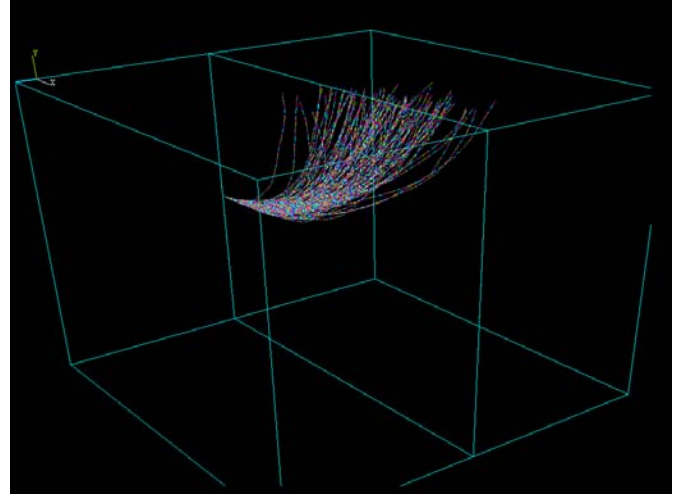


Fig.4: Test case: ion beam expanding into an upward streaming background gas, no external electromagnetic fields, $m_{ion}=1000u$, $d=1nm$, $v_{x0}=1000m/s$, $T_{gas}=300K$, $p_{gas}=0.1Pa$, $v_{y gas}=500m/s$

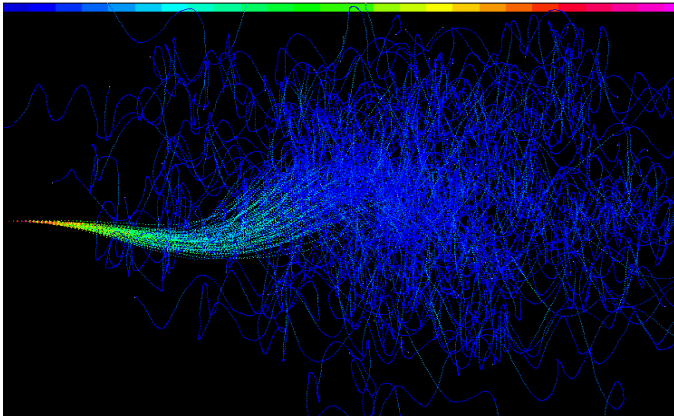


Fig.5: Test case: ion beam expanding into a resting background gas while subjected to a spatial uniform electric AC field; $m_{ion}=1000u$, $d=1nm$, $v_{x0}=500m/s$, $T_{gas}=300K$, $p_{gas}=0.1Pa$, $v_{gas}=0m/s$, $E_{yAC}=5V/m$, $f=500Hz$, $n_{coll}=5 \cdot 10^4$, color indicates ion temperature

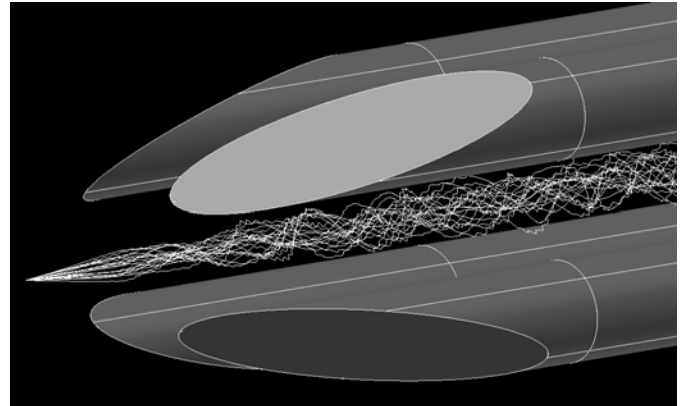


Fig.6: Ion injection into a RF quadrupole: $m_{ion}=1000u$, $f=500kHz$, $U_{AC,eff}=500V$; $\vec{v}_0 = \vec{e}_x \cdot 600m/s + \hat{\mathcal{R}} \cdot 100m/s$ some trajectories transferred back to the ANSYS post processor; notice the characteristic ion motion in the RF field

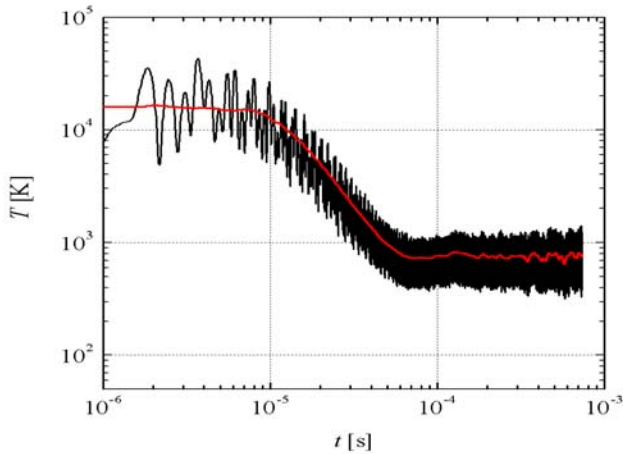


Fig.7: Thermal ion temperature as a function of time of a hot ion cloud injected into a gas filled RF quadrupole: $m_{ion}=1000u$, $d=1nm$, $T_{gas}=300K$, $p_{gas}=10Pa$, $v_{gas}=0m/s$, $|E_{max}|=10^5V/m$, $f=816kHz$: cooling occurs within $t \leq 100\mu s$, final temperature higher than gas temperature due to collisional heating

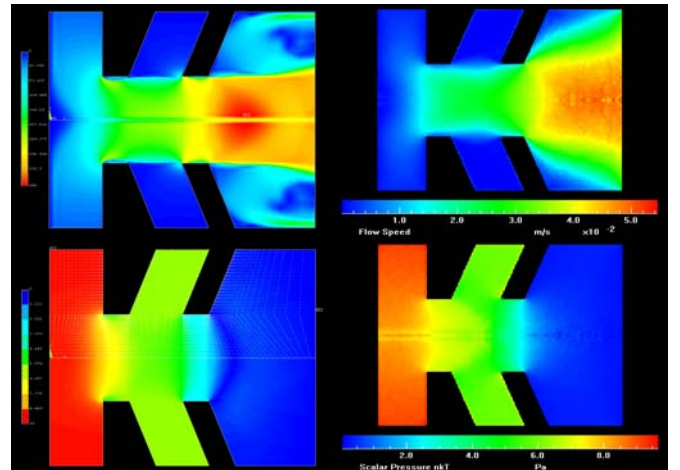


Fig.8: Comparison of Navier-Stokes (left) and DSMC solutions (right) for an axisymmetric gas expansion problem (system shown in Fig. 9): contour plots of flow velocity (top) and pressure (bottom)

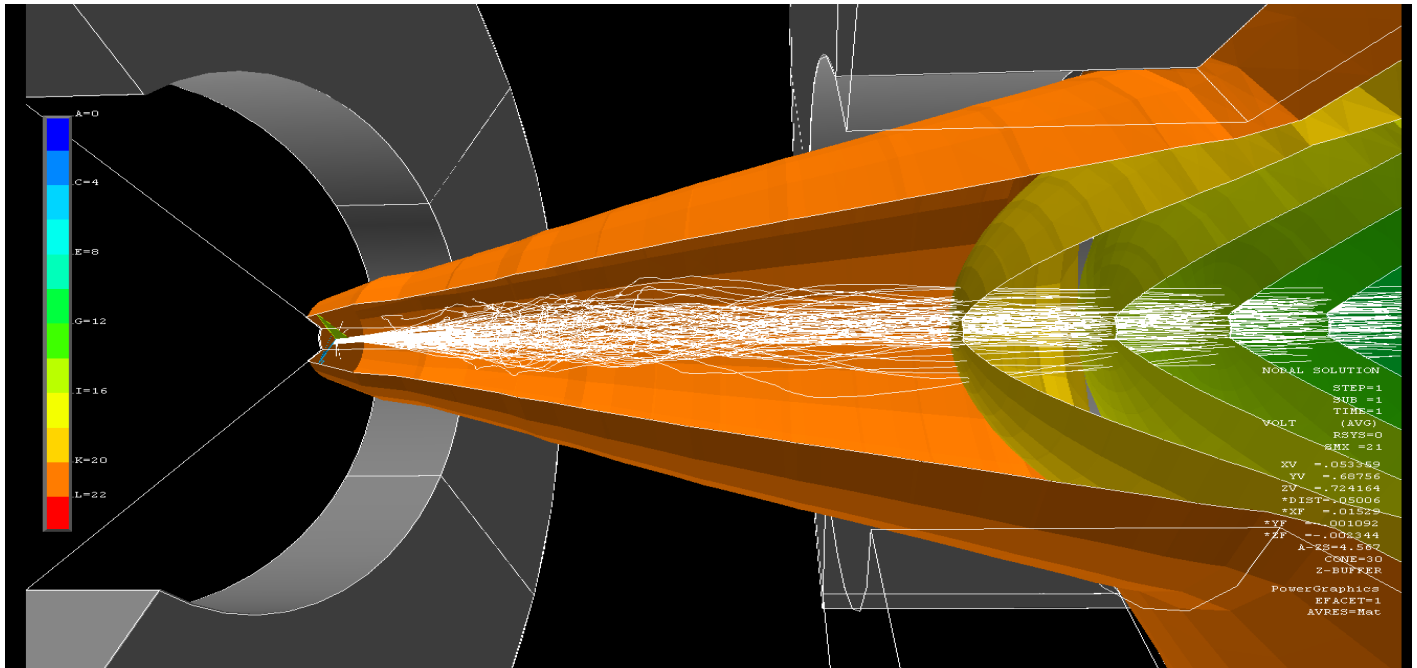


Fig.9: Early stage of an ion beam in a multi-electrode ion generation system, isosurface plot of electric potential, $m_{ion}=1000u$, $\vec{v}_0 = \vec{e}_x \cdot 1000m/s + \vec{\mathfrak{R}} \cdot 200m/s$ $d=1nm$, $p_{gas_max}=10Pa$ (computed gas flow field not displayed), $n_{coll}=5 \cdot 10^4$

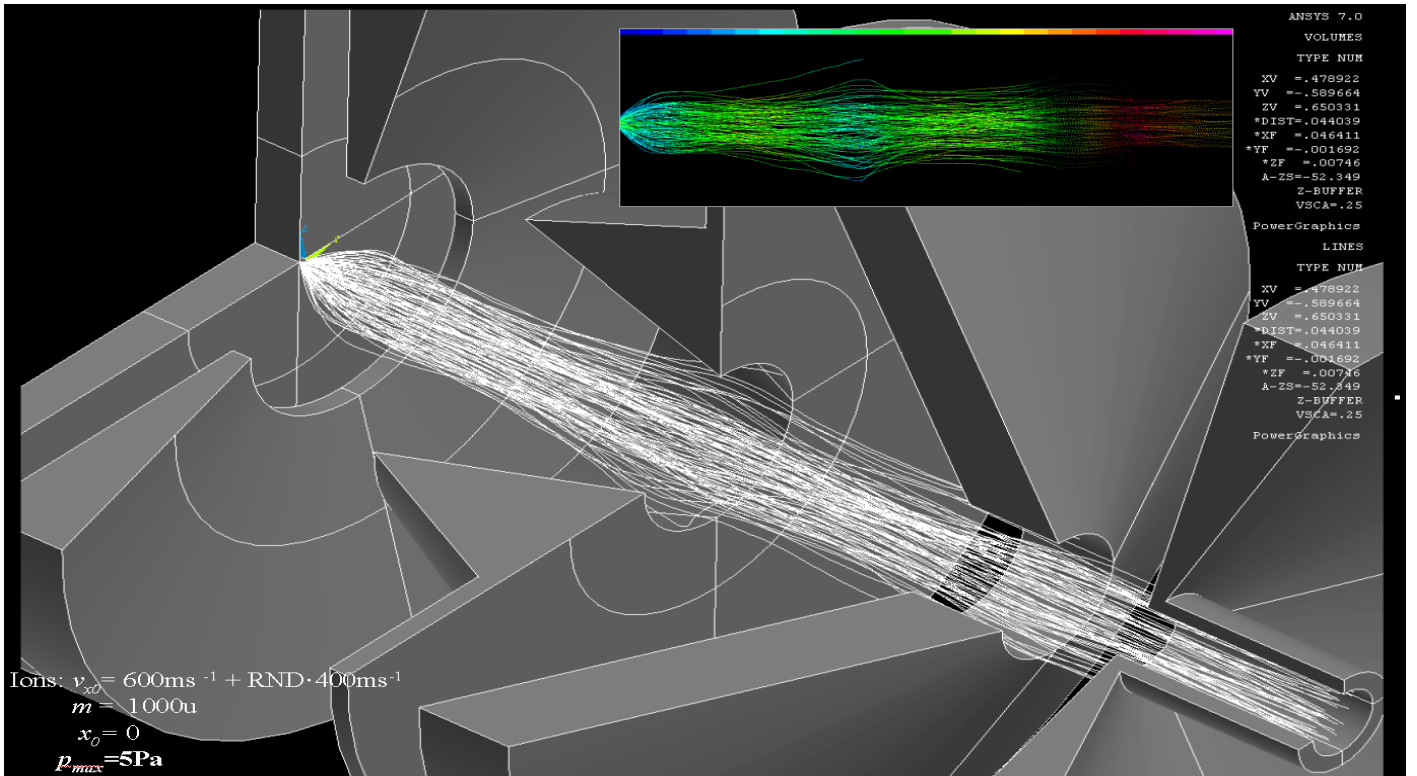


Fig.10: Ion beam in a multi-electrode ion generation system with background gas, $m_{ion}=1000u$, $\vec{v}_0 = \vec{e}_x \cdot 600m/s + \vec{\mathfrak{R}} \cdot 400m/s$ $d=1nm$, $p_{gas_max}=5Pa$, average number of collision per ion trajectory: 295, inserted picture shows trajectories colored according to local ion temperature; system exhibits ion losses on lenses under displayed conditions

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