Virtual Device™ 21.1

## Geometry definition, data analysis, and supersonic gas flow CFD for SIMION®.

KOLTRAN LABS

Virtual Device, developed by Koltran Labs (Dr. Sergei Koltsov), is an add-on package for SIMION. Its **Light version** provides additional convenient ways of defining electrode geometries for SIMION and analyzing/plotting SIMION data recording output. A more advanced **Hydrodynamics version** also contains a unique gas flow (CFD) solver for supersonic jets (e.g. ESI sources) and a corresponding SIMION 8.1 collision model.
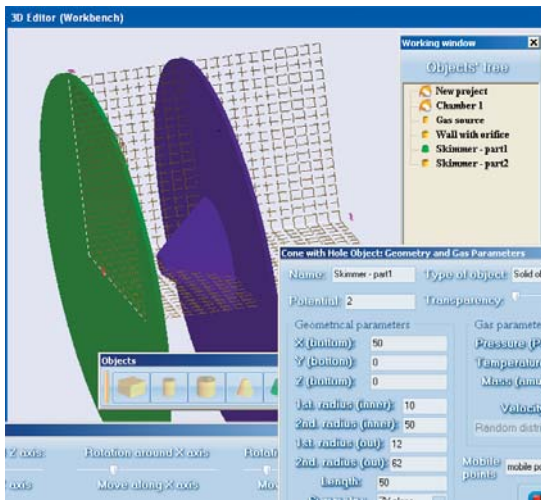

Electrode geometries and boundary conditions

can be defined with the **3D Editor** program included in both versions of Virtual Device. This is a **graphical CAD-like program for composing complex electrode geometries** from a set of basic shapes like spheres, cones and bars. Models can be exported as geometry files (.**GEM**) for use in SIMION. In the hydrodynamics version, **boundary conditions for gas flows** can also be defined in the same model and exported for CFD calculation (discussed below).

Gas flows can be calculated

in the **Virtual Jet** program included in the Hydrodynamics version of Virtual Device. This calculates gas flow around electrodes, under conditions of **supersonic, compressible flow** (e.g. supersonic jet or ESI), using a form of the **Navier-Stokes** equations, given gas flow boundary conditions previously defined by the 3D editor. The mathematical/physical **computational fluid dynamics (CFD)** model of gas flow is based on the **"large particle model,"** which permits simulating a wide pressure range (**atmospheres down to about 0.5 Pa**, or lower with future extensions).   Calculations are accelerated with **OpenMP and CUDA**. Stability can be checked with real-time graphs. The results of simulation (series of arrays with gas P/T/vel./density distributions) can be exported in **SIMION .PA** format. Turbulent flows were recently added, and slip boundary conditions will soon be released in 21.2
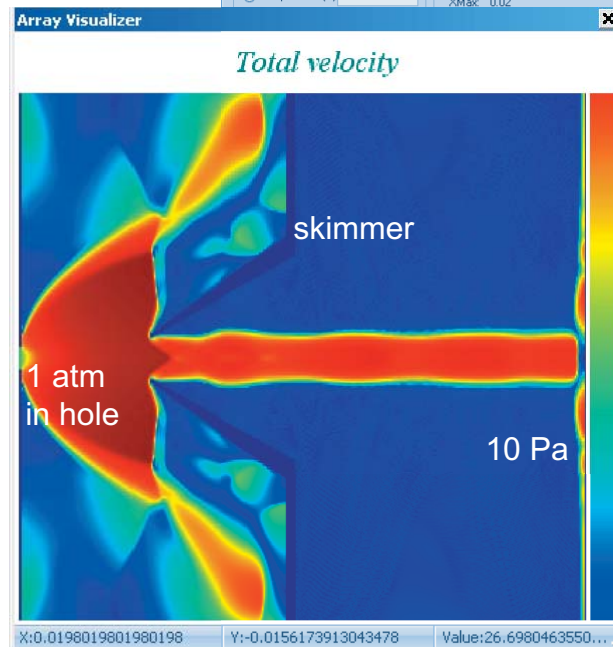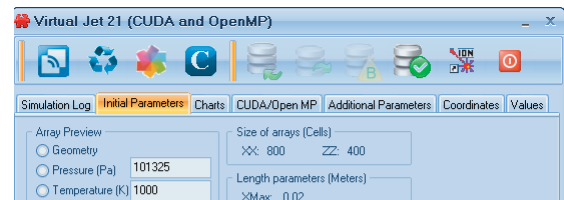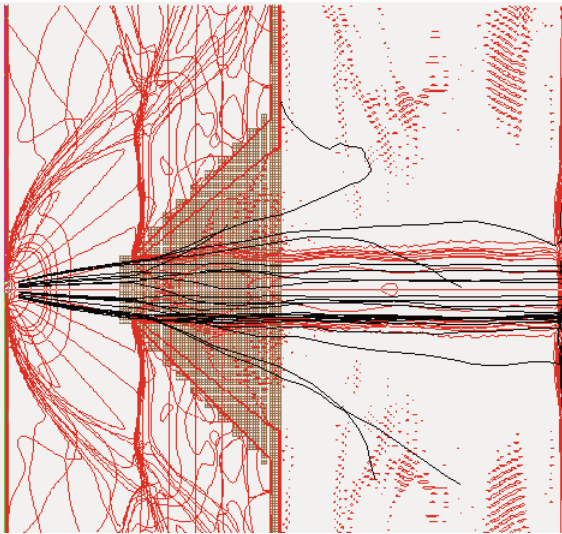
Particle trajectories in gas flows

can optionally be calculated in conjunction with SIMION 8.1. The Hydrodynamics vesion of Virtual Jet provides a **user program** (Lua code), which can be loaded into SIMION to model ion-gas collisions with a 3D background gas flow distribution defined in **PA files** previously calculated by Virtual Jet. Gas flows can be visualized by usual SIMION 8.1 methods. A detailed manual on the model theory is provided, with emphasis on ESI related applications.

Data analysis and graphing

can be done using the **Data Analysis program** included in both versions of Virtual Device. This directly reads **SIMION data recording output** files and can do ion distributions, phase distributions in different planes, histograms of exit parameters (for estimating peak shape), transformation of time of flight into mass/charge terms, and calculation of mass resolution. Data can be transformed into Excel format. The new version supports multi-event analysis.
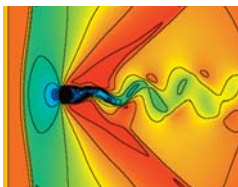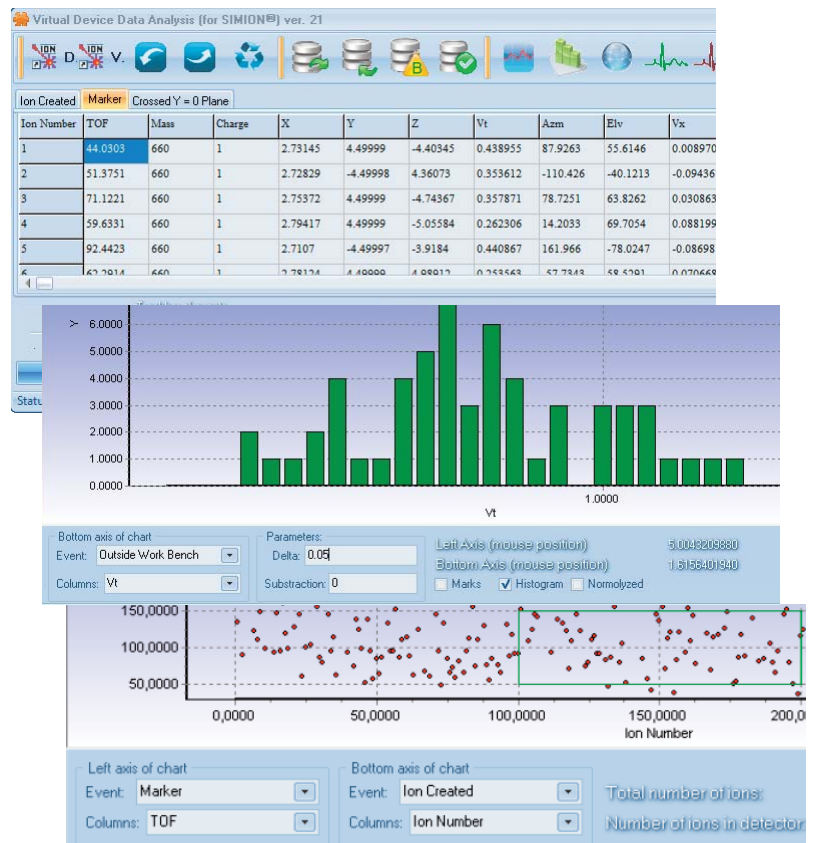
For more details see http://simion.com/virtualdevice

A free limited demo version (with hydrodynamics) is available from the "Check for Updates" button in SIMION 8.0/8.1.

Part No.	Description	Price
SIMIONV	Virtual Device 21.1 Light	
SIMIONVH21	Virtual Device 21.1 Hydrodynamics	