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Introduction

Mass spectrometry (MS) is one of the main tools for detecting chemical or biological components, where gas dynamics interfaces play a crucial role for delivering ionized components from the atmosphere directly into the low-pressure area.

The visualization of gas flow inside interfaces provides fruitful information about gas dynamics processes; that information can be used for tests of numerical schemes.

We use Volume Ray Casting² technology for visualization of gas flow, where the simulation is based on the Large Particle Model proposed earlier¹.

Algorithm of visualization

In this work, we propose an algorithm of visualization, which consists of the three stages:

1. Modeling gas flow based on the Large Particle Model. Resulting from the simulation is a series of arrays that contains 3D distribution of gas parameters.

Each cell in these arrays is regarded as a voxel (a 3D volume element, analogous to the 2D term 'pixel'). The content of cells is used for calculation of color intensity in 3D visualization.

2. Computations. The cell intensity can be transformed with a 1D color lookup table so each cell is associated with a color and transparency (red, green, blue, alpha), which allows to make certain parts of the 3D scene visible or invisible.

This helps project the intensity at each voxel location to the front panel with the corresponding levels of red, green and blue colors, and intensity. In addition, for each cell we pre-compute the gradient, where the change in the cell's intensity relative to its neighbors is codes as a surface normal with intensity (X,Y,Z, intensity).

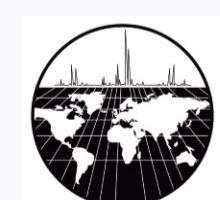
3. Calculation of each voxel color intensity in 3D scene. It is based on casting the rays through the volume from the back to the front.

This is analogous to a projectile being fired through the volume from the location of each screen pixel. As the projectile traverses the volume it accumulates the color of the material it penetrates.

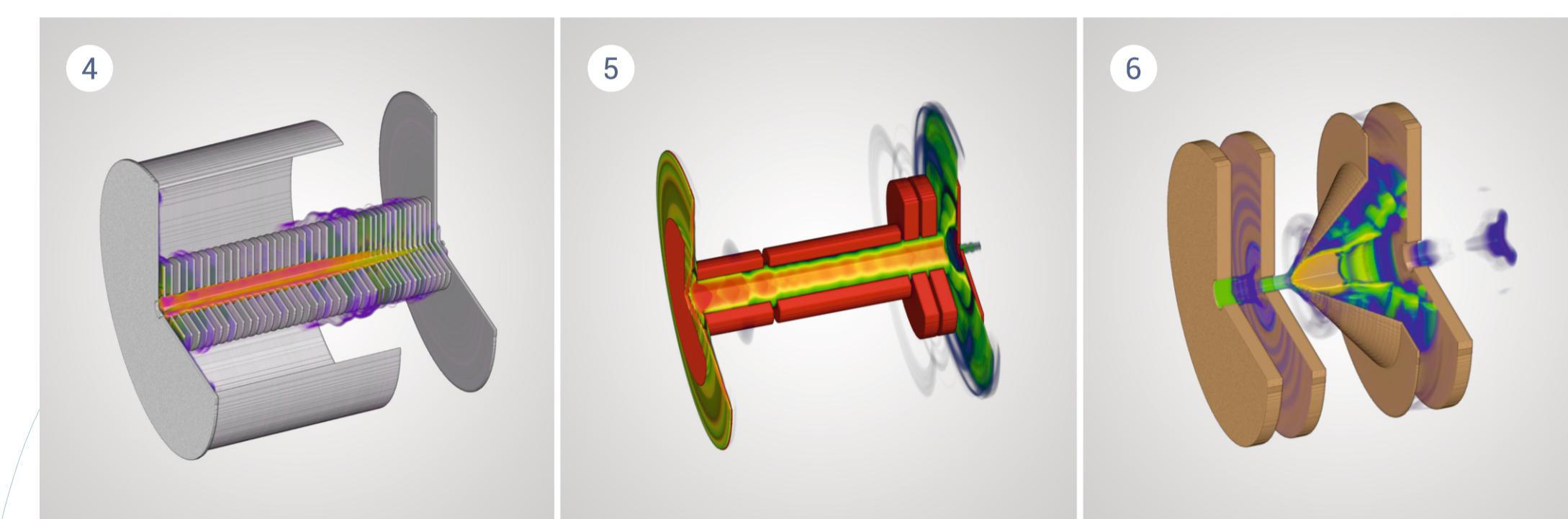
4. Adjusting transparency based on gradient magnitude. In addition to the basic material properties, the ray is modulated by the gradient intensity. Such approach is known as Edge coloring³.

This highlights interfaces where the velocity changes rapidly. For example, the density of shock waves in a supersonic jet differs significantly from that in the plane flow of gas, therefore by setting up a threshold of the voxel intensity, our algorithm provides extraction of the 3D Mach disk structure and the large turbulent whirlwinds.

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Picture 4. Example of a gas flow through a set of electrodes with different holes (velocity distribution)

Picture 5. Example of gas flow in nozzle-skimmer, skimmer - quadrupols and steering plates regions

Picture 6. Example of gas flow through regions with different pressure (KUNSHAN HEXIN MASS SPECTROMETRY)

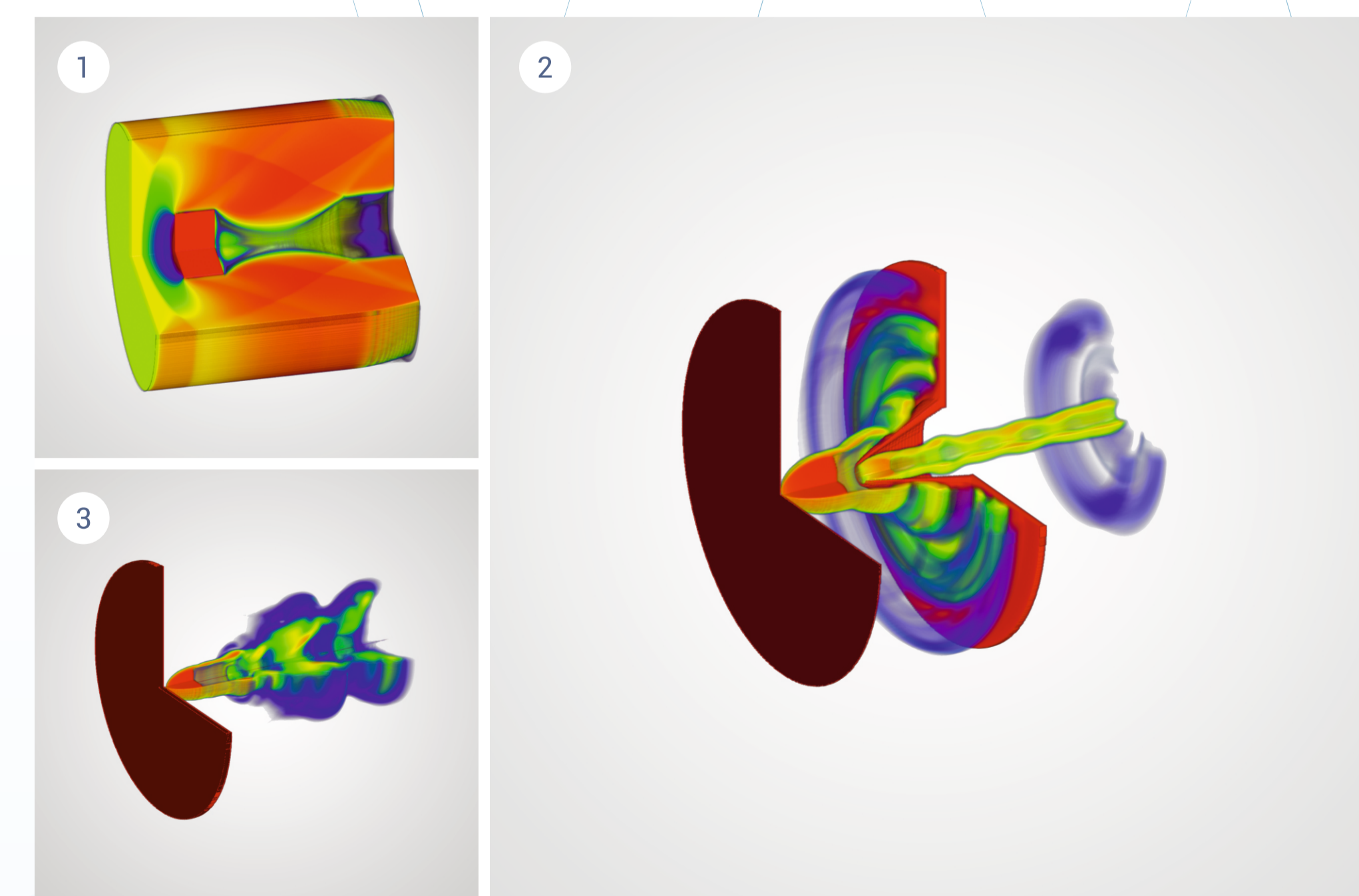
Conclusion

We propose a combination of the Volume Ray Casting technology and the Large Particle Model for simulation and interactive visualization of gas flow inside of gas dynamic interfaces. The project uses the open source project MRICROGL (<http://www.cabiati.com/mricro/raycast/>).

By using OpenGL's GLSL shader language this program can run all of the popular desktop operating systems (Windows, OSX, Linux) and on commodity hardware from any of the popular vendors (Intel, AMD, NVidia).

Literature

1. Sergey Koltsov, Clemens Walther. Application of electrospray mass-spectrometry for nanoparticle investigations: Simulation of ion movement in a supersonic jet, Online Proc. 17th International Mass Spectrometry Conference, ThP-016 (2006).
2. Min Chen, Arie E. Kaufman, Roni Yagel (Eds), "Volume Graphics".
3. Brandon Ellenberger, K. Evan Nowak, Non-Photorealistic Real-time Volume Rendering, <http://pages.cs.wisc.edu/~nowak/779/779ClassProject.html>



Picture 1. Example of turbulent flow

Picture 2. Example velocity distribution in ESI interface

Picture 3. Example of Mach disk