# Simblend - an open source visualization toolchain for SIMION

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## Introduction

The charged particle simulator **SIMION** [1] is among the most commonly used numerical tools in the mass spectrometry community. Despite its capabilities, SIMION lacks flexible, high-quality visualization methods. For many applications, particularly for educational purposes, an appropriate and visually appealing presentation of the simulation results is desirable.

The open source tool **Blender** [2] is a powerful 3D modeling and rendering system. It allows the generation of very high quality still image visualizations and animations.

To combine SIMION with Blender, we have developed a plugin (named **Simblend**) which imports simulated ion trajectory data from SIMION into Blender

## Software Modules



The Simblend plugin was newly developed by IPAMS in a student project
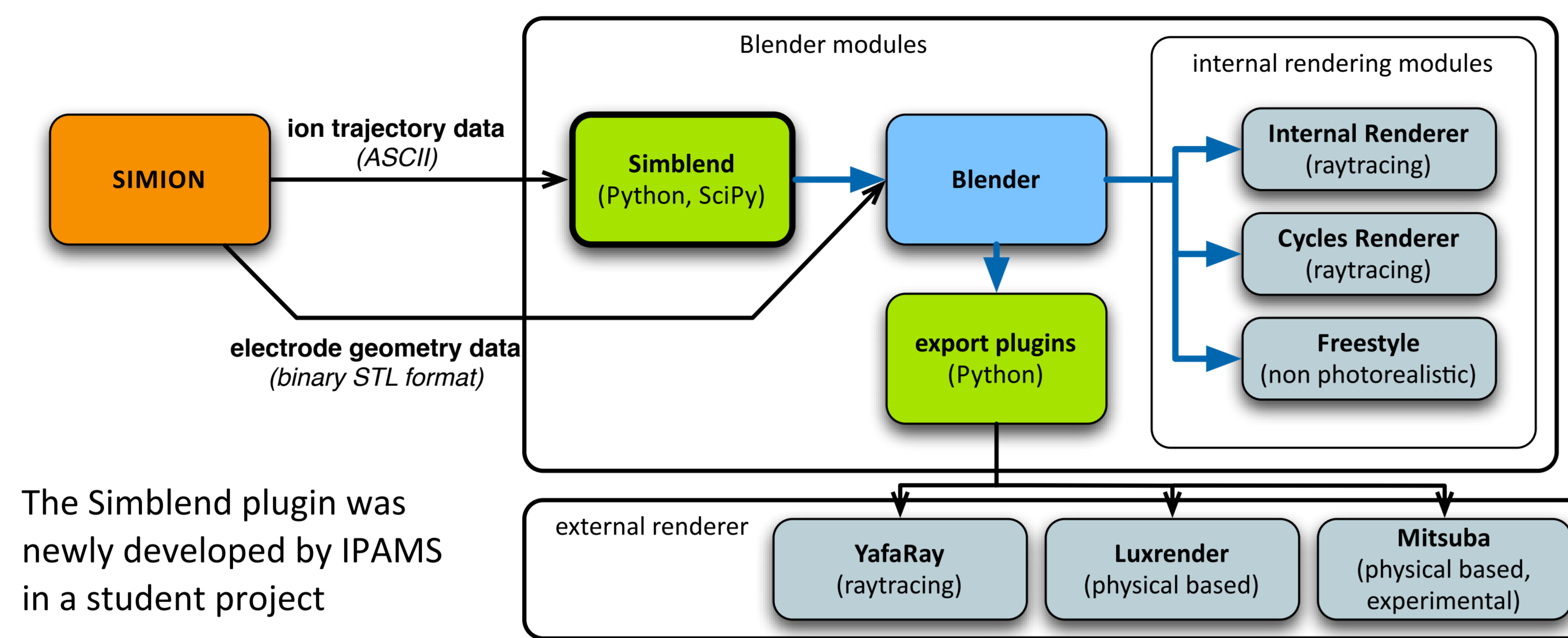
## Simblend import plugin

**Basics:**
Simblend is a plugin written in Python for the internal Blender API.

It takes ion **trajectory data** (ion positions, ion kinetic energy etc.) from SIMION and generates a **geometric representation** of it in Blender.

Electrode geometries can directly be exported by SIMION and imported by Blender in STL binary format (surface polygon representation).

**Trajectory representations:**
Simblend provides multiple representations of ion trajectories in Blender:

- **Sphere:** Simulated ions are presented as animated spheres
- **Tubes:** Simulated ion traces are presented as tubular streamlines. Parameters of the ion (e.g. kinetic energy) can be represented by material parameters.
- **Particles:** Simulated ions are presented as particles of the Blender particle system, which allows effects like smoke traces

## Blender

**Basics:**
Blender is a full featured, open source modeling, animation and rendering system.

It provides very sophisticated tools and features on a similar level as commercial 3d graphics packages (e.g. 3ds Max, Cinema 4D, Maya).

Its **open plugin system** has attracted an active community and allows the rapid development of import plugins like Simblend.

**General features:**
- **Python plugin system, open API** Blender is open source and has a completely open API.
- **Sophisticated animation system** Keyframe based animations, parameter interpolation / parameter curves, large number of animated ions are possible.
- **Sophisticated rendering system** Capable internal renderers (Cycles engine, Blender internal renderer, Freestyle) and external rendering systems are available.

**Rendering options:**
- **Ray tracing** Renderer provides many material options and special effects (e.g. transparent materials, reflections, volumetric materials).
- **Physical based rendering** Accurate physical based lighting for very high quality photorealistic renderings.
- **Non-photorealistic rendering** Line style graphics and renderings resembling technical or artistical drawings are possible.
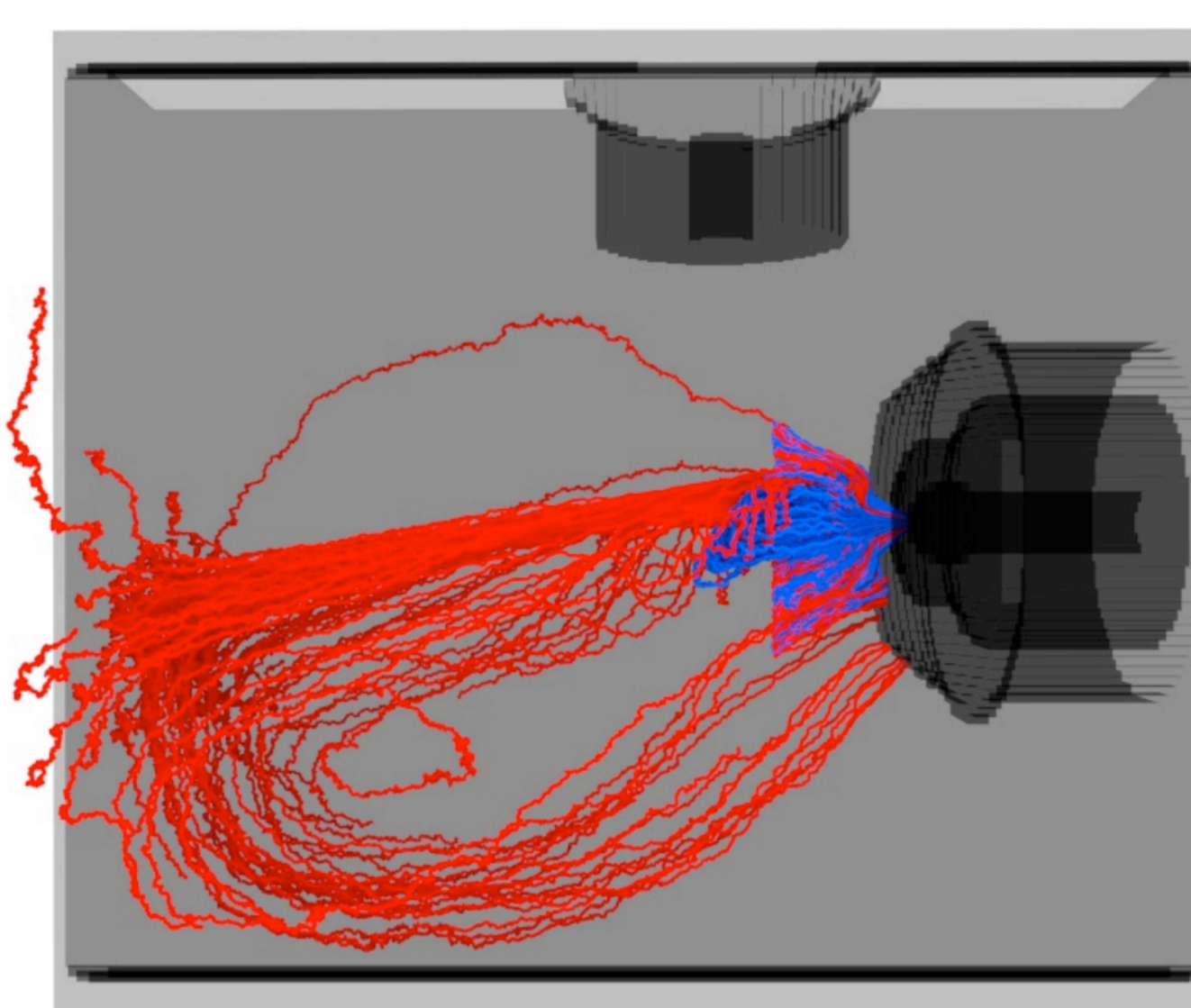
## Exemplary visualizations

### Ion trajectories in AP ion source: Ray tracing
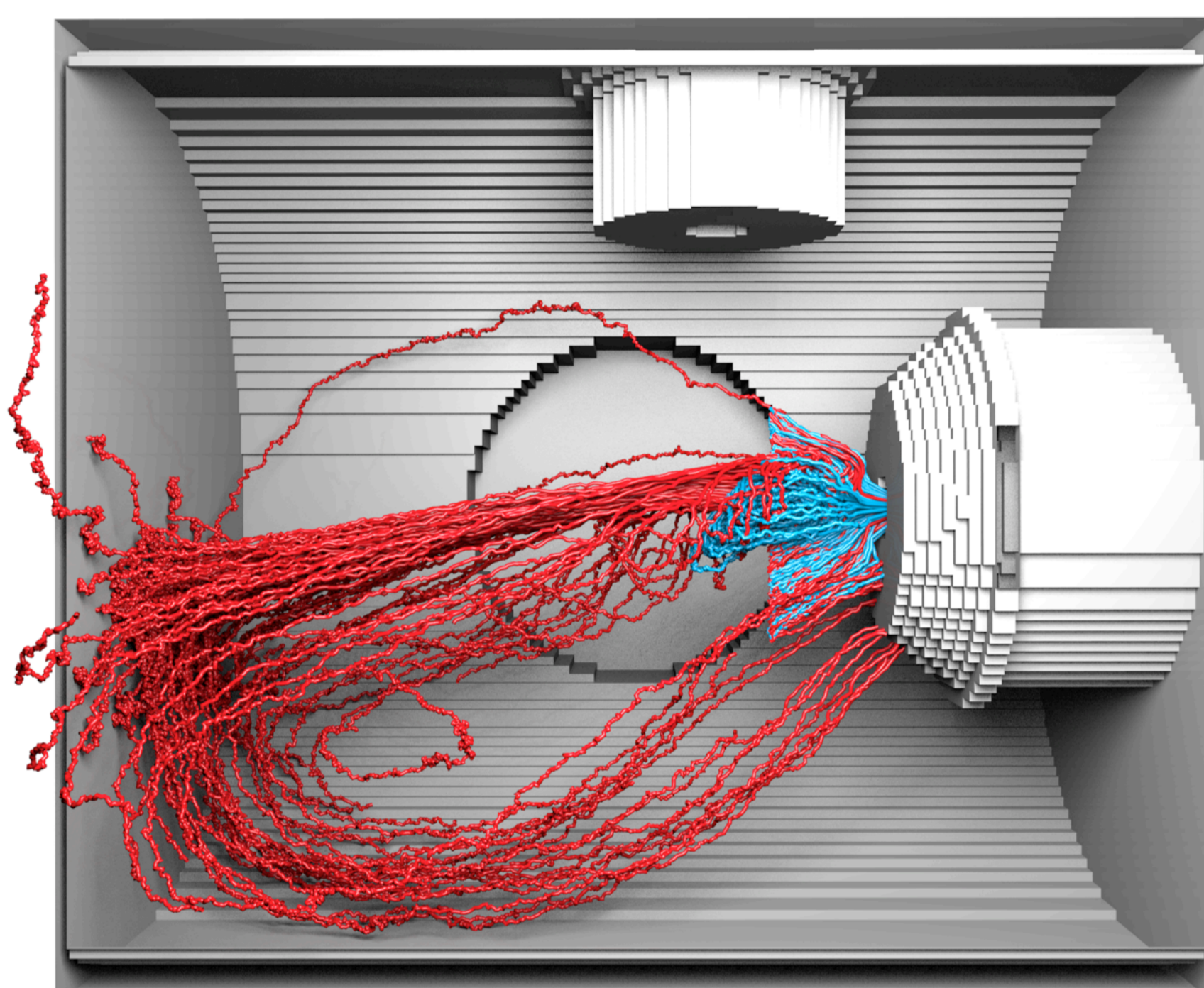


**left:**
Ion trajectories in an AP ion source (MPIS) rendered with the internal Blender renderer.
A section of the source chamber has been removed (cut) to allow the view inside.

**Blue trajectories:**
Low dry-gas flow (2.0 l/min)
**Red trajectories:**
High dry-gas flow (3.8 l/min)

### Ray tracing options



**above:**
The same data presented left, rendered with Cycles. The electrode geometry is shown semi-transparent.
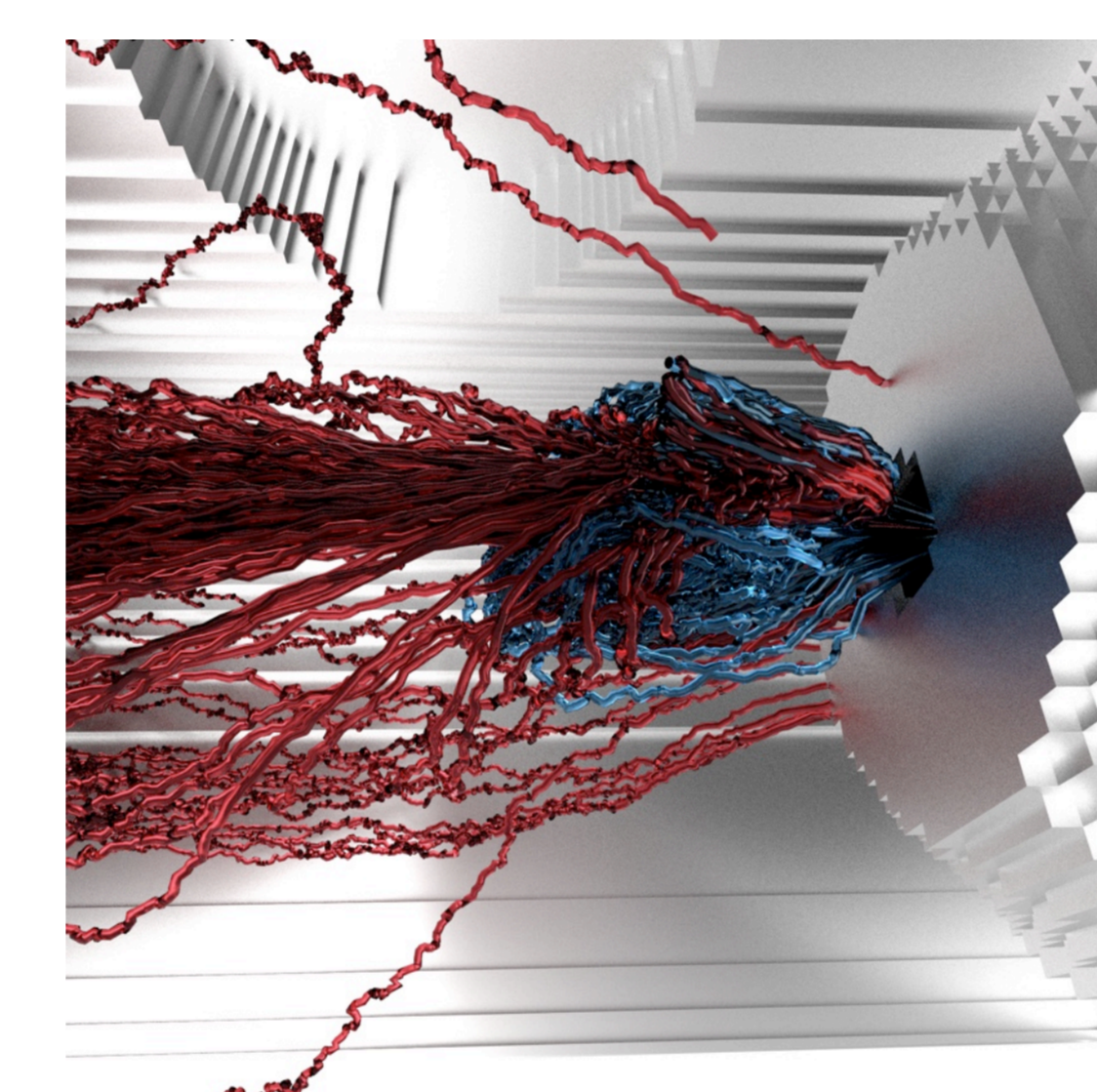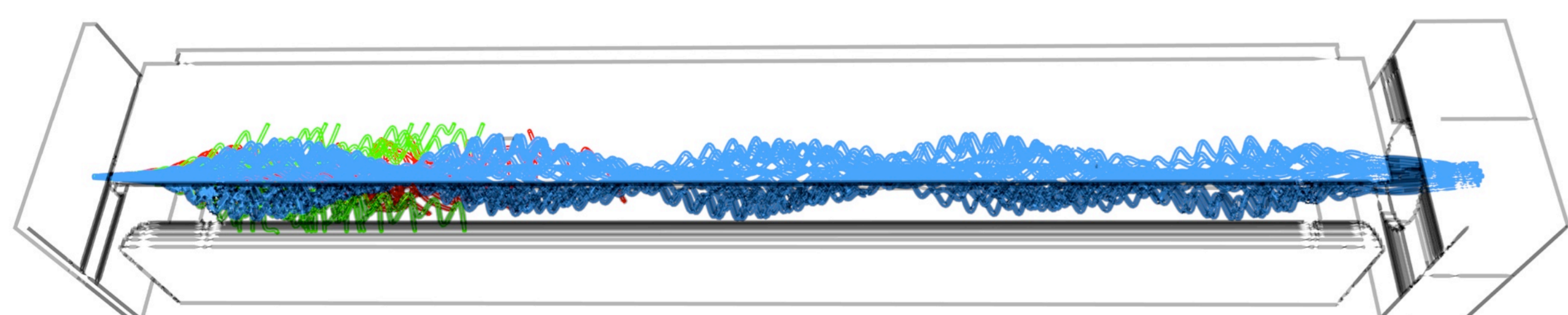
**above:**
Detailed view of the data, rendered in Cycles with photorealistic glass and metal materials.

### Ion trajectories in a quadrupole: Non-photorealistic rendering

The **Freestyle** module of Blender allows the generation of non-photorealistic line renderings, which are demonstrated here with the quadrupole example of SIMION.
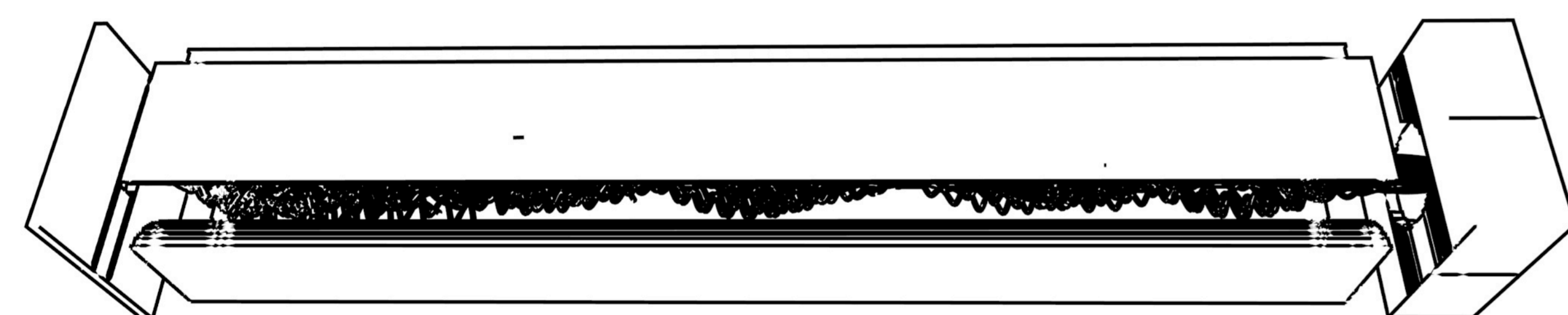


**above:**
Basic outline rendering. Edges of the geometry are presented as line drawing, hidden lines are not rendered.

**above:**
Outline rendering. Edges of the geometry are presented as line drawing, hidden lines are rendered with an individual, lighter line style. Ion trace edges are drawn in ion group colors according to the ion mass.

### Artistic renderings

Freestyle provides many line style effects which allow artistic renderings of electrode geometries and ion trajectories.
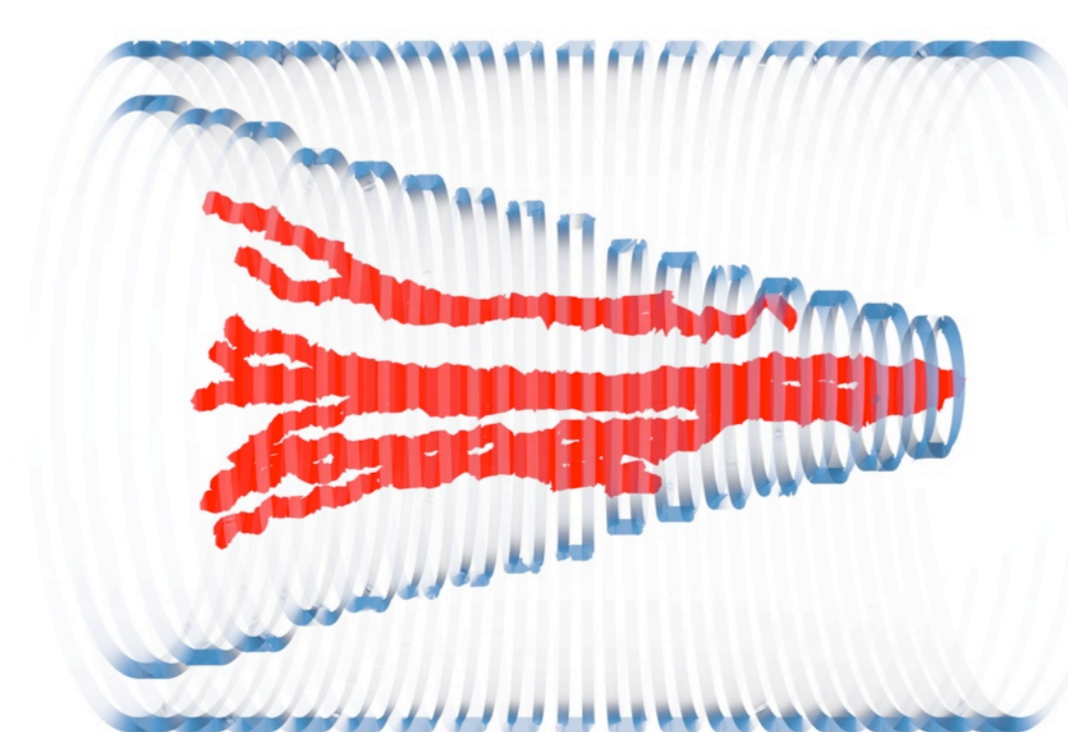


**right:**
Non-photorealistic rendering of an ion funnel geometry with ion trajectories depicted in red
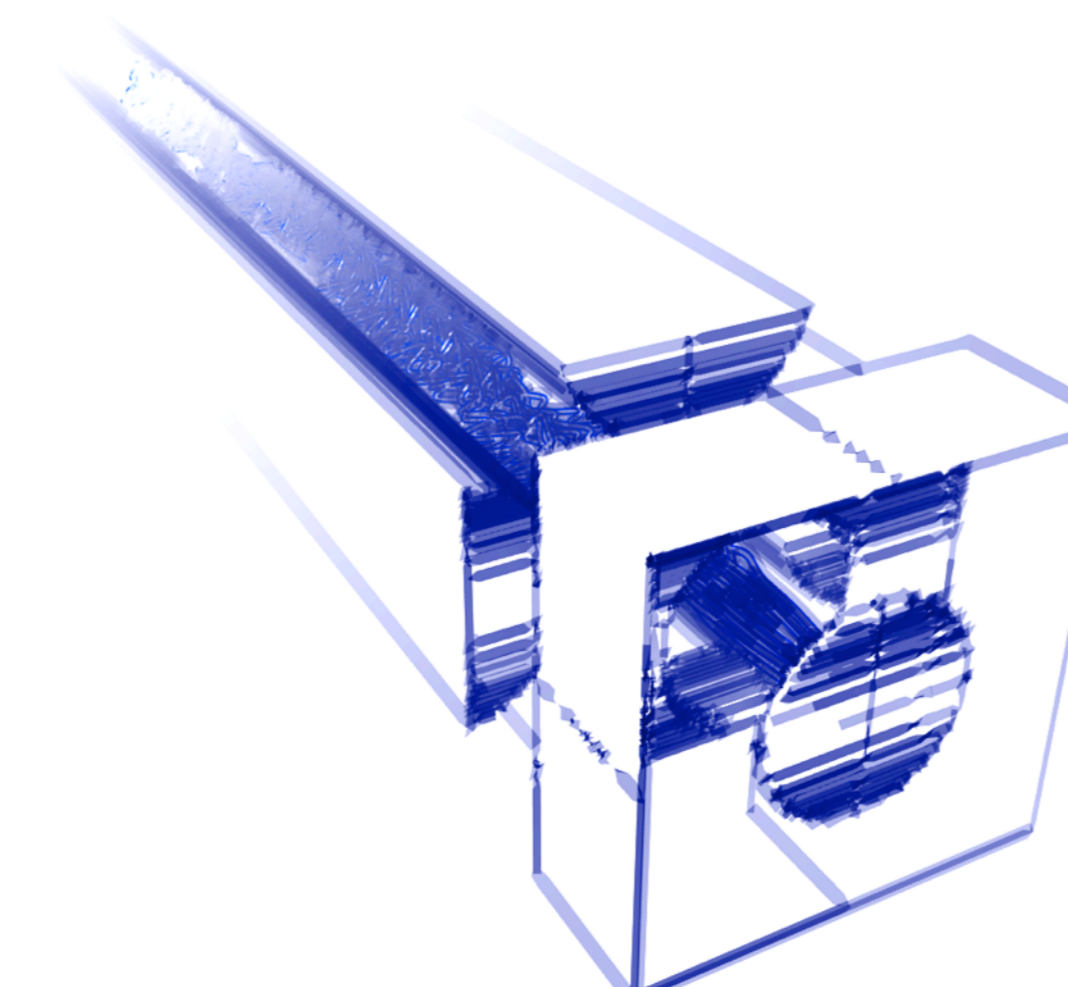
**right:**
Artistic line rendering of the quadrupole geometry

## Simblend import options

### Ion paths
Ion trajectories can be imported as tubular paths. Individual ion masses may have individual material settings.

In the example on the right the kinetic ion energy is depicted as light emission of the tube material.
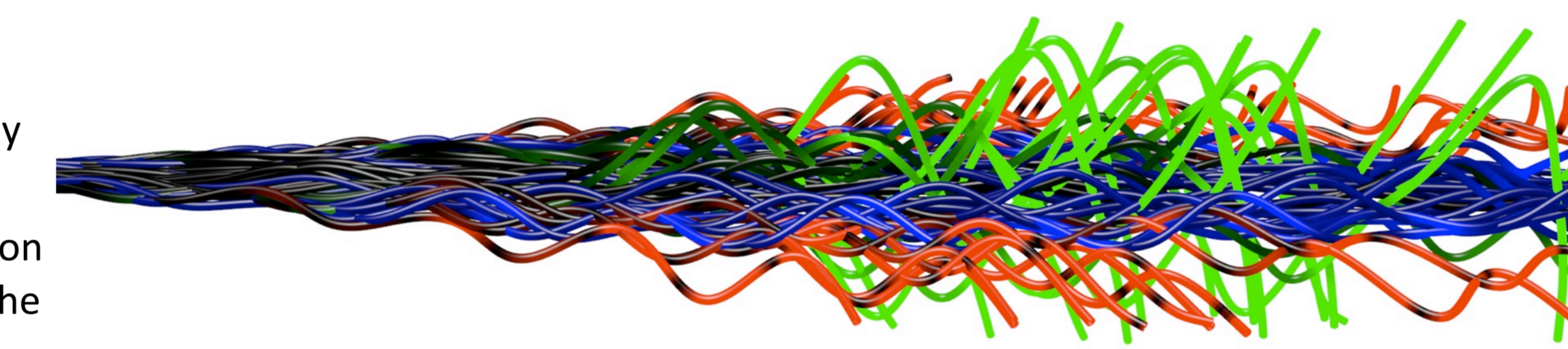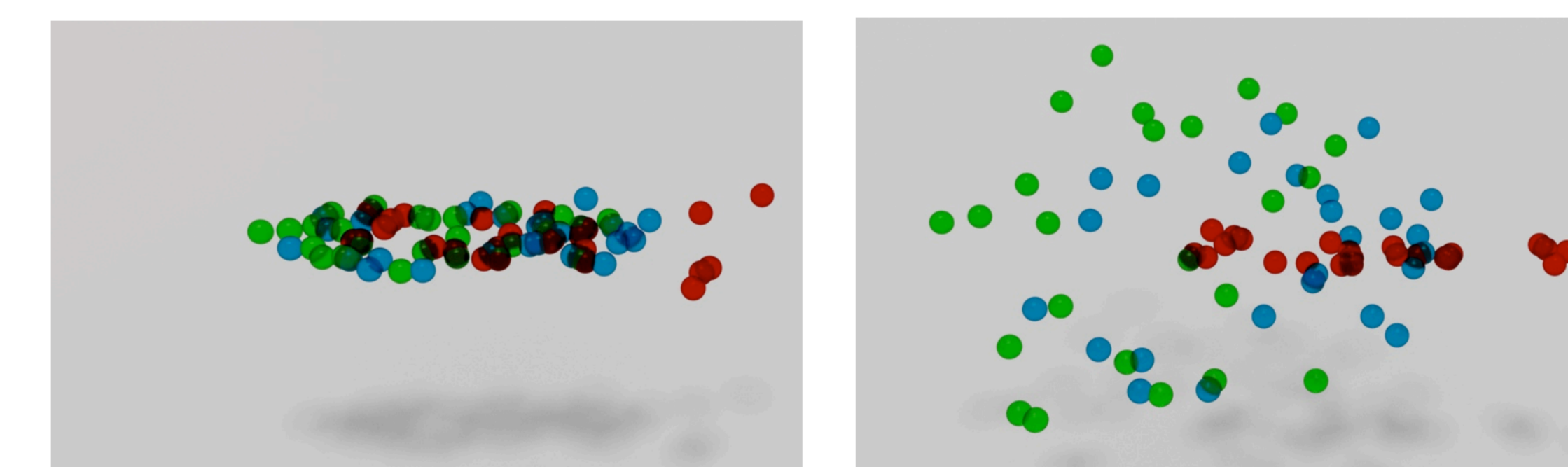


### Ions as particle system emitter
Ions can be imported as emitters for the Blender particle system. This allows effects like smoke or light trails.

In the example on the right ion paths are depicted as light emitting particle traces with a color and a transparency gradient along the trace.
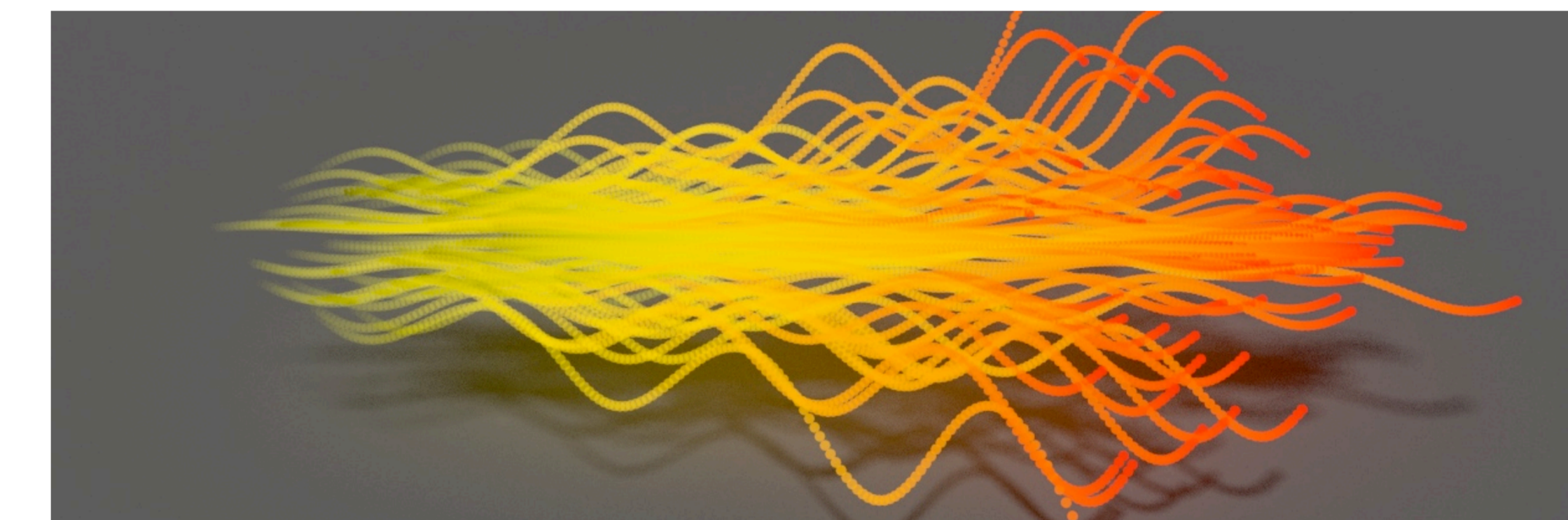


### Ions as spheres
Ions can be imported as spheres with individual material settings. This is primarily feasible for rendered animations, when particle systems are not appropriate or too expensive in terms of rendering time.



## Simblend trajectory import parameters



**Original trajectories**
- Example trajectories show strong random component from the gas collision model
- No trajectory smoothing
- Default path-tube diameter
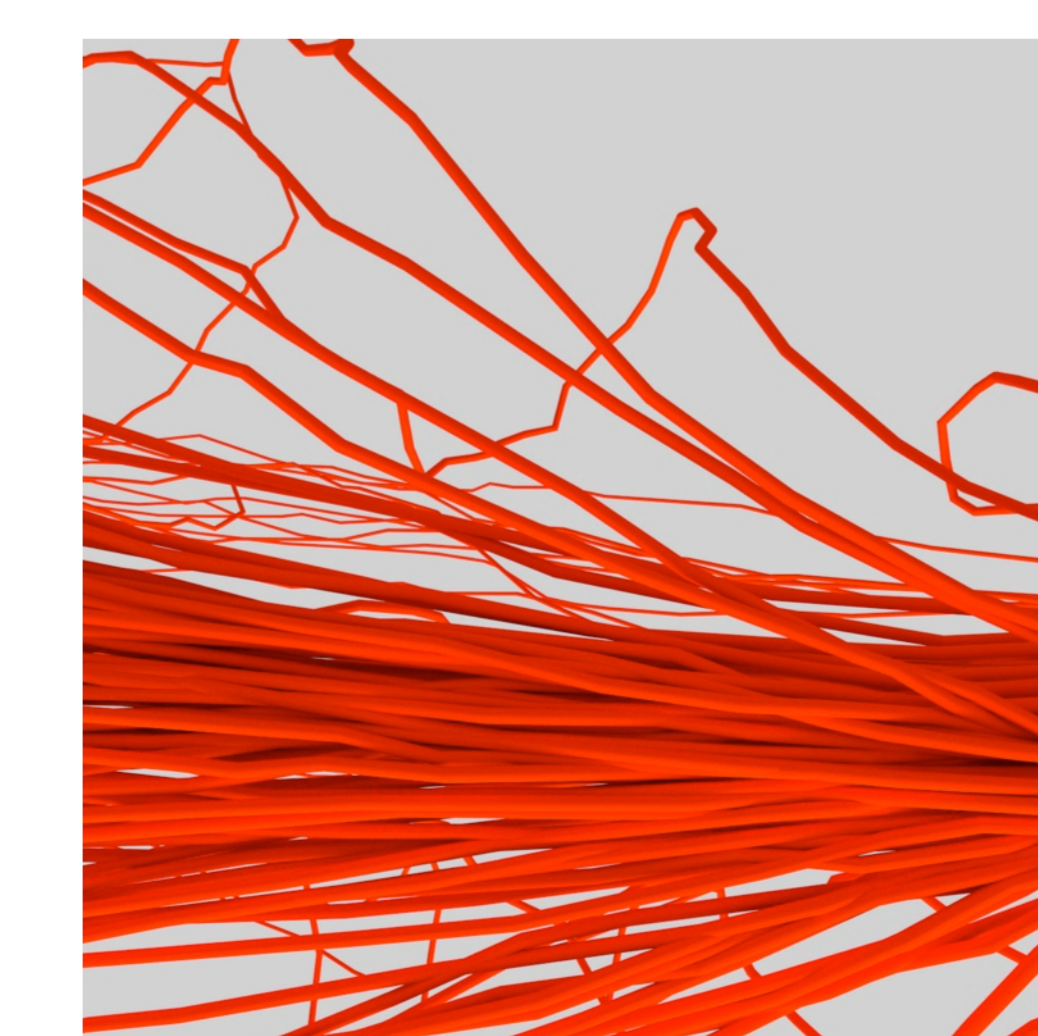
**Trajectory smoothing**
- Ion trajectories can be smoothed by Simblend which also reduces the complexity of the tubes
- Default path-tube diameter
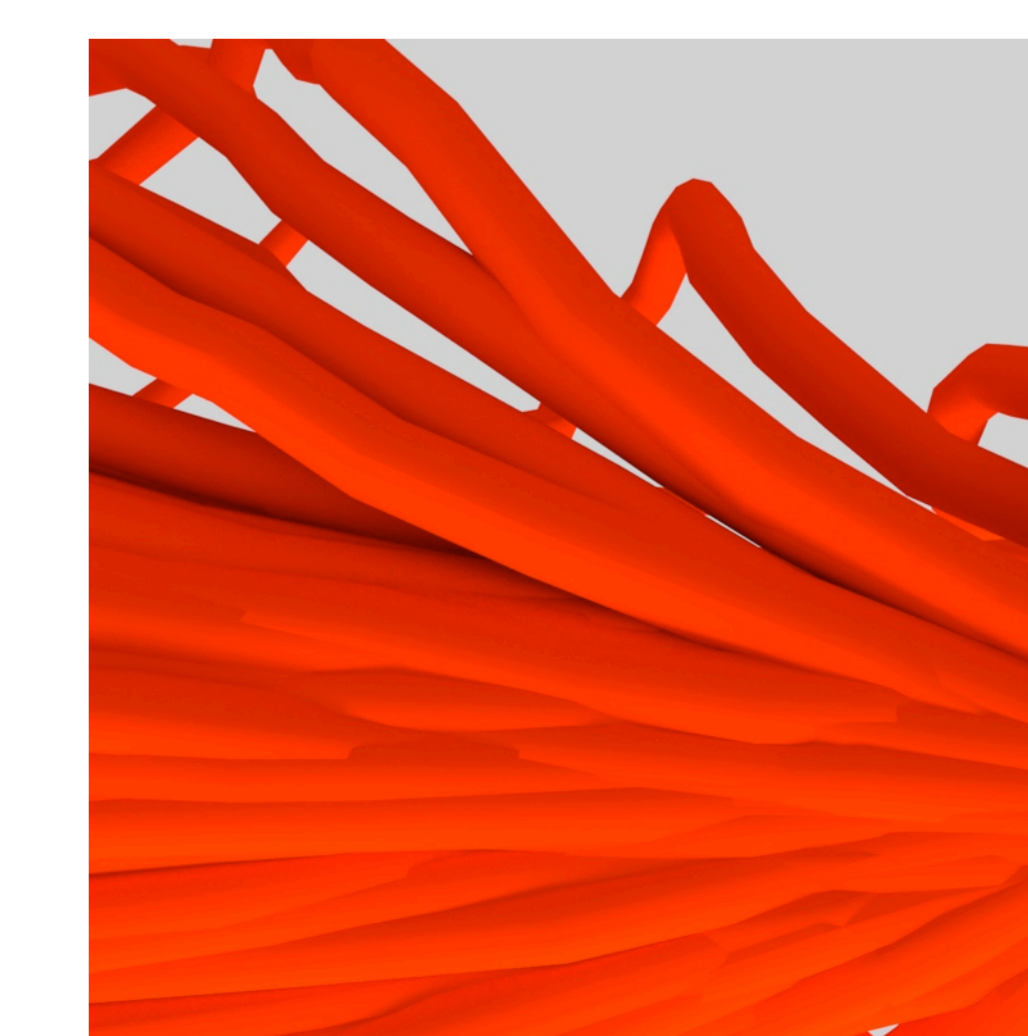
**Path tube radius**
- The radius of the tubes can be adjusted
- Naturally the radius has to be appropriate for the individual visualization
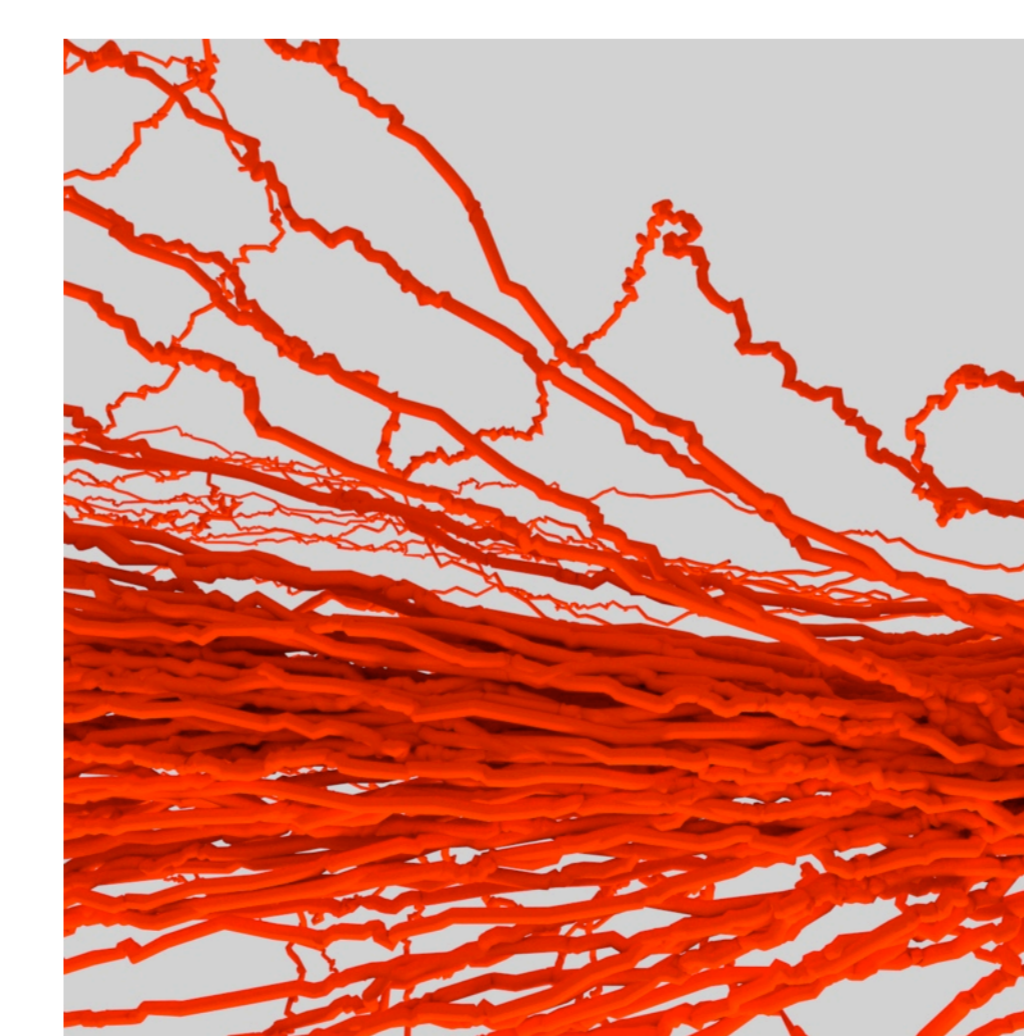
## Conclusions

**Results:**
- Simblend allows the import of calculated ion trajectories from SIMION
- Electrode geometry import into Blender is possible via STL
- The ion trajectory import and rendering (still images and animations) can be performed on modern consumer class computer hardware
- For special renderings and rendered animations, Blender ideally extends the capabilities of SIMION

**Outlook:**
The existing state of Simblend is a first step. Further development will include:
- More import options in Simblend
- Better integration of the geometry import into Simblend
- Feasible presets, e.g. for materials, or particle systems

## References

[1] Scientific Instrument Services Inc., SIMION 8.1
http://www.simion.com

[2] Blender community, Blender 2.67
http://www.blender.org

[3] Python community, Python programming language
http://www.python.org

[3] NumPy community, NumPy numerical computing package
http://www.numpy.org

[4] Luxrender community, Luxrender
http://www.luxrender.org

[5] YafaRay community, YafaRay,
http://www.yafaray.org

## Acknowledgement