User's Guide

<u>Starfish</u>

2D Plasma / Gas Simulation Program

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Contents

I. Introduction

Starfish is a two-dimensional XY/RZ plasma and gas simulation code written in Java [1]. The code was developed with generality in mind, allowing it to consider a wide range of gas dynamics problems. The current version mainly implements functionality needed for simulations of low-density plasmas using the Particle In Cell Method (PIC) with MCC/DSMC collisions. Rudimentary support for fluid modeling is also implemented and we are working on extending this functionality as soon as possible. Starfish operates on structured 2D Cartesian or body fitted stretched meshes. Surface geometry is included via linear or cubic splines. The code is easily extensible using plugins, as described later in this document.

Starfish consists of two version. The Light Edition (Starfish-LE) is the main code described in this document. It implements numerical models needed to perform simple gas kinetics simulations. The binary and source code for this version can be downloaded by visiting https://www.particleincell.com/starfish. The full version (Starfish-Full) implements various proprietary models mainly for modeling ion sources and surface interactions. The full version is not publicly available.

I.a)   License
Please review **LICENSE** included with the code. Your use of the code implies consent to the license agreement. In general, you are allowed to use the code for any non-commercial purpose assuming the original copyright notice is preserved.

I.b)   Getting Started
Although we started working on the GUI, a working version of GUI is not yet available. For now, Starfish is run from the command line. You need to have a Java Run Time[1] environment installed on your system. To use the code, navigate to the directory containing the simulation input files. To run the code, type
java -jre <path_to_starfish-LE.jar>
For instance, if your starfish-LE.jar file is located in a folder "codes/starfish-LE" in your home directory, and if the case you wanted to run was located in a subfolder "dat/tutorial/step1", you would do the following:
> cd starfish-LE
> cd dat/tutorial/step1
> java -jar ../../../starfish-LE.jar

Figure 1. Starfish running on Microsoft Windows in Windows PowerShell (left) and Cygwin (right)

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[1] Java JRE can be downloaded from https://java.com/en/download/

Figure 1 shows Starfish running on Microsoft Windows with the Windows Powershell (an update to the command promp) and the Linux emulator Cygwin. Note, we do not recommend running large Starfish cases from within Cygwin. At least as of this writing, Cygwin does not expose all CPU cores to the running processes and thus running Starfish from within Cygwin will result in the code running in serial.

I.c)   Input File Structure

When Starfish launches, it looks for a file called **starfish.xml** located in the current directory. This is an XML file containing multiple tags in the format
<simulation>
<tag>...</tag>
<tag>...</tag>
</simulation>

Any text enclosed with **<!--** and **-->** is considered a comment. For instance:
<!-- this is a comment -->
<tag> ... </tag>

Each "tag" corresponds to a Starfish command. The full listing of available commands is given in Section VI.

II. Numerical Model

Starfish is based on the concept that in gas simulations, we are interested in simulating the evolution of density, velocity, and temperature of one or more gaseous materials. In general, any time dependent gas simulation can be reduced to the following pseudo code:

```
for (it in num_time_steps):
    for (material in list_of_materials):
        material.integrateByDt()
```

The "integrateByDt()" function simply advances the material bulk properties in time by a simulation time step Δt. What this function actually does is specific on the type of material and the type of simulation we are interest in running. For instance, for low density plasmas, this step may involve advancing simulation macroparticles by Δt using the Particle In Cell (PIC) method [2]. For dense neutral gases, a Navier-Stokes solver may be used instead. The Starfish-LE version implements the PIC method as well as a rudimentary advection-diffusion solver. Additional material types may be added in the future. In the PIC method, the gas is represented by a number of simulation macroparticles. Each macroparticle corresponds to some w_{sp} number of real molecules, ions, or electrons. This approach is needed, since it is not computationally feasible to track every single real molecule outside some limiting low-density, tiny domain cases. Despite Starfish being a 2D code, each particle retains three components of position and velocity. The out-of-plane position is used to rotate the particle back to the computational slice in axisymmetric simulations. Particle positions in the simulation plane are then used to compute number density of material "i" n_i by scattering particle positions to a computational grid. In case of charged simulations, we next compute charge density $\rho = \sum_i^{mats} n_i$. Poisson's equation, $\epsilon_0 \nabla^2 \phi = -\rho$ is then used to obtain plasma potential, which is in turn used to compute the electric field, $\vec{E} = -\nabla \phi$. Particle velocities are updated from Lorentz force, $\vec{F} = q(\vec{E} + \vec{v} \times \vec{B})$. Starfish uses the Leapfrog integrator with the Boris scheme used for the velocity update.

III. Examples

III.a)   Flow of plasma past a charged cylinder

We demonstrate the use of Starfish by summarizing a tutorial that was previously posted to the PIC-C blog[2]. In this simulation we will investigate the flow of plasma over an infinitely long charged cylinder.

Step 1: Computational Domain and Initial Field

We start the tutorial by specifying the computational domain, loading the problem geometry, solving plasma potential, and outputting results. No particles are introduced yet. The output that we will generate is shown in Figure 2.
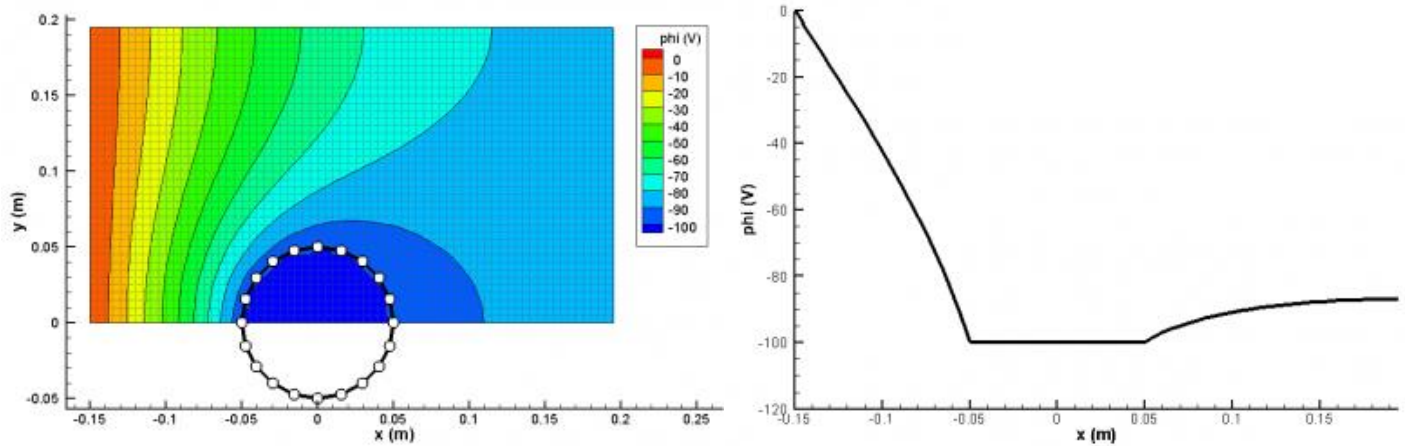
Figure 2. The initial plasma potential on a 2D mesh and as a slice along Y=0.

As noted earlier, Starfish looks for a file named starfish.xml located in the current directory. This file contains all the commands that drive the simulation. The file used to produce the above output is shown below:

```
<simulation>

<note>Starfish Tutorial: Part 1</note>

<!-- load input files -->
<load>domain.xml</load>
<load>materials.xml</load>
<load>boundaries.xml</load>

<!-- set potential solver -->
<solver type="poisson">
<n0>1e12</n0>
<Te0>1.5</Te0>
<phi0>0</phi0>
<max_it>1e4</max_it>
</solver>

<!-- set time parameters -->
<time>
<num_it>1</num_it>
<dt>1e-6</dt>
```

[2] https://www.particleincell.com/2012/starfish-tutorial-part1/

```
</time>

<!-- run simulation -->
<starfish />

<!-- save results -->
<output type="2D" file_name="field.dat" format="tecplot">
<scalars>phi, efi, efj, rho, nd.0+</scalars>
</output>

<output type="1D" file_name="profile.dat" format="tecplot">
<mesh>mesh1</mesh>
<index>J=0</index>
<scalars>phi, efi, efj, rho, nd.o+</scalars>
</output>

<output type="boundaries" file_name="boundaries.dat" format="tecplot" />

</simulation>
```

As you can see, this file is an XML document and it contains a number of elements nested within the parent **<simulation>** element. We will now review these commands in detail

Line 2: <note>

The input file starts with the note command, which simply outputs the specified message to the screen and the log file. This is a convenient way to remind you what simulation case the code is running.

Lines 5-7: <load>

The file next contains three load commands. These commands load the specified file and place it into the XML tree at the current position. They are used to split a single input file into more manageable smaller chunks. This command is particularly handy for data reuse, for instance, to reuse commonly used material definitions and material interaction tables. We will go through the content of these in more detail below.

Lines 10-15: <solver>

Lines 10 through 15 contain the solver command. This command is used to specify the details of the solver that will be used in the simulation. Here we use the non-linear Poisson solver. The parameters specify the reference values for the Boltzmann electron model, as well as the maximum number of iterations for the linear solver. Other parameters can also be set, such as the tolerance, and the settings for the non-linear NR solver, but here we just use the defaults. You can see the value of these by looking in the log file.

Lines 18-21: <time>

We next set time control parameters. We tell the code to run for a total of zero iterations. We also specify the time step size, which in this case is ignored. Running for zero iterations instructs the code to solve the initial field, but it will not attempt to inject particles (assuming sources were defined).

Line 24: <starfish>
On line 24 we finally start the simulation with the starfish command. All commands before this one were simply specifying the inputs, now these are used to compute the solution. The input file parser will wait for the solver to finish before moving to the next command.

Lines 27-37: <output>
By itself, the starfish command does not produce any useful output. The computed results are stored internally in memory and must be saved to the output file for post-processing. This is done with the output command. Three types of output are supported: 2D, 1D, and Boundaries. The first saves data on the 2D computational mesh. The 1D type is similar but it saves only a subset of the mesh, one with a fixed I or J coordinate. The Boundaries output saves data along the simulation geometry. This plot is useful for outputting surface-type parameters such as erosion rate or surface flux. Here we use it to simply save the loaded object geometry.

Domain File (domain.xml)
We now return to line 5, and consider the domain specification. The domain file, **domain.xml**, contains the following:

```
<domain type="xy">

<mesh type="uniform" name="mesh1">
<origin>-0.15,0</origin>
<spacing>5e-3, 5e-3</spacing>
<nodes>70, 40</nodes>
<mesh-bc wall="left" type="dirichlet" value="0" />
<mesh-bc wall="bottom" type="symmetry"/>
</mesh>

</domain>
```

One of the unique features of Starfish is its ability to load an arbitrary number of computational meshes (**note this functionality is broken in 0.18 but is being worked on)**. These meshes can be either rectilinear or body fitted elliptic meshes. In this example, we specify just a single rectilinear mesh. We first tell the code that our geometry is in the Cartesian (XY) coordinate system. Starfish also supports axisymmetric (RZ) domains. The uniform Cartesian mesh is specified by providing the location of the origin, node spacing, and the number of nodes in the two coordinate directions. We also apply a mesh boundary condition by setting the left wall to a fixed 0V potential. This is needed in order to create a potential gradient between the ambient free space and the sphere. We also let the bottom face be symmetric since we are simulating only one half of the computational domain.

Materials definition (materials.xml)
Starfish does not contain any build database of materials or material interactions. This information must be provided by the user. Since we don't have any particles in this first step, we don't yet concern ourselves with the interactions, however, we need to define the materials that will be present in the simulation. The materials file contains the following:

```
<!-- materials file -->
<materials>

<material name="O+" type="kinetic">
<molwt>16</molwt>
<charge>1</charge>
<spwt>5e9</spwt>
<init>nd_back=1e4</init>
</material>
```

```
<material name="SS" type="solid">
<molwt>52.3</molwt>
</material>

</materials>
```

As you can see, we defined two materials: atomic oxygen ions and stainless steel. The atomic oxygen ions are kinetic. This material will be modeled with simulation particles within the particle in cell method. Starfish also supports fluid materials, which use Navier Stokes or MHD equations to propagate densities, as well as solid materials, which don't change throughout the simulation. The parameters needed to specify a material will depend greatly on its type. For the kinetic oxygen ions, we specify the particle specific weight, the number of real particles each simulation macroparticle represents. This number will influence the number of simulation particles in the simulation. We also specify the background density. A non-zero background density is required whenever the Boltzmann electron model is used due to the presence of the logarithmic term.

Geometry file (boundaries.xml)
The final piece is the geometry file boundaries.xml, which is listed below:

```
<boundaries>

<boundary name="cylinder" type="solid" value="-100" reverse="false">
<material>SS</material>
<path>M 0.05, 0 L 0.0475528, -0.0154508 0.0404508, -0.0293893 0.0293893, -0.0404508
0.0154508, -0.0475528 -9.18E-18, -0.05 -0.0154508, -0.0475528 -0.0293893, -0.0404508 -
0.0404508, -0.0293893 -0.0475528, -0.0154508 -0.05, 6.12E-18 -0.0475528, 0.0154508 -
0.0404508, 0.0293893 -0.0293893, 0.0404508 -0.0154508, 0.0475528 3.06E-18, 0.05
0.0154508, 0.0475528 0.0293893, 0.0404508 0.0404508, 0.0293893 0.0475528, 0.0154508
0.05, 0</path>
</boundary>

</boundaries>
```

Currently, simulation objects are specified via linear or cubic Bezier splines. It is possible that a future version of the code will include elementary building-block shapes and support for other file formats. The boundary contains a child field called path which provides the geometrical information about the spline. The syntax is similar to the SVG format, with the exception that cubic splines are specified by simply listing the points through which the spline will pass and the control knot points are omitted. Here we use linear components (L) to trace a circle. The ordering of the nodes matters, since the code will use the ordering to figure out which side of the segment is "internal" to the object. The internal side is assumed to lie on the "left", hence the circle segments move counter-clockwise. This path was created with the included MakeCircle.java program.

Mesh Generation
Finally, a quick note about mesh generation. Right now, Starfish supports just the "staircase" or "sugarcube" method. The code simply uses the provided surface boundary to figure out which mesh nodes are internal, and these nodes are given the boundary condition of the surface spline. A more detailed method of using cut cells is still in development. You can see in Figure 3 below the staircasing effect. This plot is generated by visualizing the "type" data field. The nodes in red as flagged as internal and the ones in blue comprise the gas domain. It is important to check that node location was set correctly before launching the simulation.
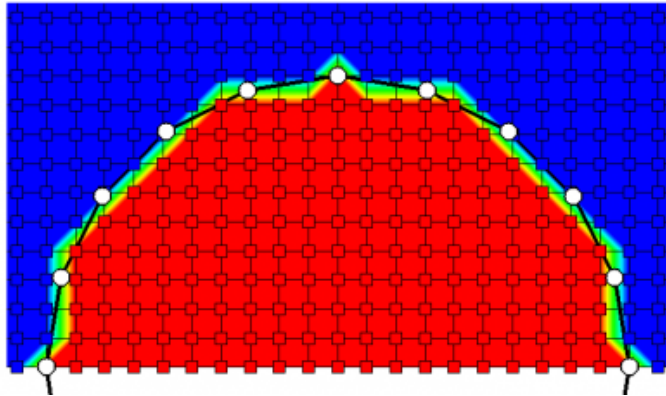
Figure 3. Internal nodes (in red) set with the sugarcubing algorithm

Step 2: Particles and Animation

We now add particles to our simulation. In order to add particles, we need to specify sources. Starfish supports two types of sources: volume and surface. Here we will use the latter. Surface sources create particles along geometry **(boundary)** splines according to a prescribed velocity distribution function (VDF) and the surface normal vector. In this example, we want the entire left domain boundary to act as a source injecting particles with uniform velocity. This setup then approximates the movement of the cylinder through undisturbed plasma, with the frame of reference moving with the cylinder. First, we need to add a new boundary to the boundaries.xml file:

```
<boundaries>

<boundary name="cylinder" type="solid" value="-1" reverse="false">
<material>SS</material>
<path>...</path>
</path>
</boundary>

<boundary name="inlet" type="virtual" >
<path>M -0.15,0.2 L -0.15, 0</path>
</boundary>

</boundaries>
```

We named this spline "inlet" and it was given a type of virtual. This classification means that the boundary will not be used in generating the mesh intersections nor will it be seen by the particles. It is available for use by sources and also by probes (but more about probes later). This spline is simply a linear segment from the bottom left to the top left corner of the computation mesh. As you can see, it is 0.2m long.

To add the source, we add the following command to starfish.xml (this command could also be placed in an external file and loaded with the <load> command):

```
<!-- set sources -->
<sources>
<boundary_source name="space">
<type>uniform</type>
<material>O+</material>
<boundary>inlet</boundary>
<mdot>5.313e-11</mdot>
```

```
<v_drift>10000</v_drift>
</boundary_source>
</sources>
```

Here you can see how the boundary comes into play. The source is given type uniform, which means that it produces particles with velocity equal to v_drift. The particles will be moving in the direction of the surface normal of the associated boundary, the inlet. If the boundary consisted of a number of individual splines, the particles would be moving according to the local normal. This source will generate O+ particles at mass flow rate of 5.313e-11 kg/s. You may be wondering how this number was determined. We want our plasma density in the free space to be 10^{12} m^{-3} to correspond with the potential solver electron model settings. The mass flow rate is given by the following expression:

$$\dot{m} = mnuA$$

where the terms on the RHS correspond to the atomic mass (16 amu, per materials.xml file), number density (1e12 m^{-3}), velocity (10,000 m/s), and source area (0.2 m^2). In the Cartesian (XY) mode, the area is equal to the spline length, since unit depth is assumed. This expression gives us the value that is used in the simulation. Also, since we now have particles, we need to run for enough time steps to reach the steady state. In this case, 400 time steps will do the trick. We modify the time command as follows:

```
<!-- set time parameters -->
<time>
<num_it>400</num_it>
<dt>2e-7</dt>
</time>
```

After you run the simulation, we obtain results like those visualized in Figure 4 and Figure 5 . We can see that a wake forms behind the cylinder. We can also clearly see the "reflection" of ions at the centerline, the line of symmetry. In reality, this reflection corresponds to the influx of particles from the opposite half of the simulation. This is best seen in the plot of the vertical velocity.
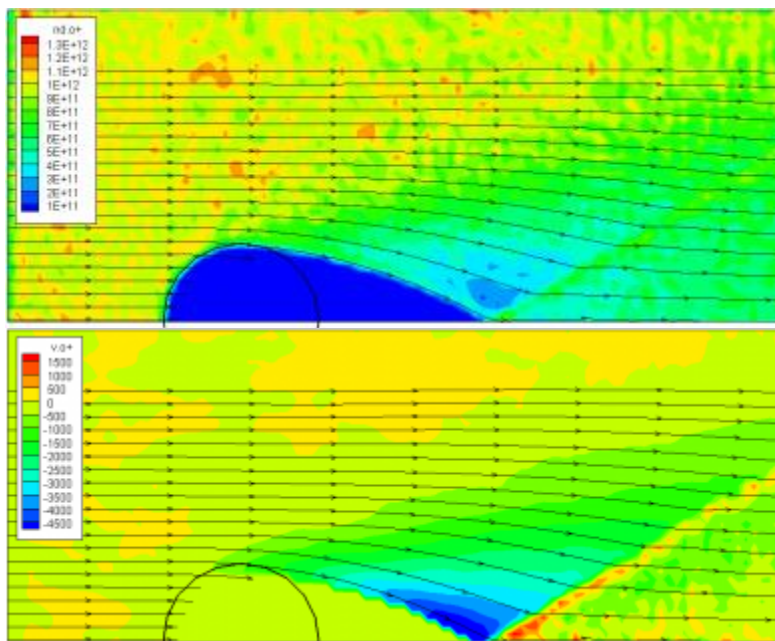

*Figure 4. Ion density and ion vertical velocity*
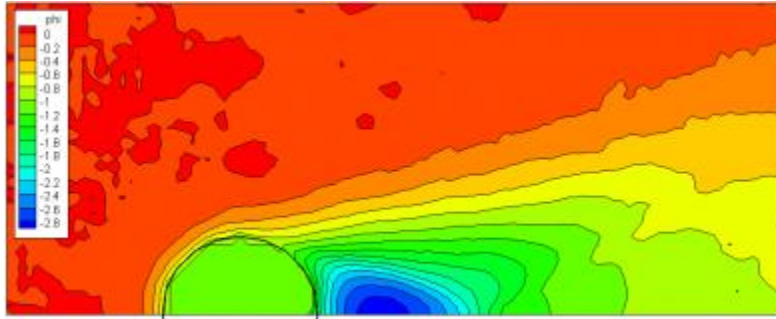
Figure 5. Plasma potential for flow over a cylinder

These results show the final solution at the end of the simulation. These results correspond to the instantaneous steady state results. But what if we wanted to learn more about how the solution progressed? Or what if we had a time-dependent injection source? This is where animations come in. Animations direct the simulation to save results at a prescribed frequency during the course of the computation. Animations are specified by wrapping the standard output command in an animation command. See the website for a visualization of this data.

```
<!-- save animation -->
<animation start_it="1" frequency="20">
<output type="2D" file_name="field_ani.dat" format="tecplot">
<scalars>phi,rho, nd.O+,u.O+,v.O+</scalars>
</output>
</animation>
```

Step 3: Surface Interactions

In the previous step, ions that collided with the cylinder were simply removed from the simulation. This is the default surface interaction that occurs if no other model is defined. It is only partially realistic. In reality, when low energy ions collide with a surface, they tend to pick up an electron from the surface and recombine into a neutral. In many plasma processes, *surface recombination* is the dominant plasma loss mechanism. Recombination in the gas itself is a three body process that is negligible at densities below 1e19 m^{-3}. Although significantly lower than atmospheric pressure, this density is still several orders of magnitude higher than densities present in common space plasma applications. For instance, the ambient plasma density at the Low Earth Orbit is around 1e12 m^{-3}. So while it is true that an ion "disappears" from the simulation on surface impact, the prior simulation does not conserve mass since the reflected neutral is not added.

We now add surface recombination to our model. This is done via Starfish's *interactions* module. This module handles interactions between all materials, either kinetic (handled by the PIC method), fluid (handled by the CFD/MHD solvers), or solid (making up the surfaces). We first create a new text file in the simulation directory called interactions.xml. The content of this file is

```
<!-- material interactions file -->
<material_interactions>

<surface_hit source="O+" target="SS">
<product>O</product>
<model>cosine</model>
<c_accom>0.5</c_accom>
<c_rest>0.9</c_rest>
</surface_hit>

</material_interactions>
```

and we load this file by adding

```
<load>interactions.xml</load>
```

to starfish.xml. We also need to add a new material to the database – remember, Starfish does not contain any built-in materials. We add the following to materials.xml:

```
<material name="O" type="kinetic">
<molwt>16</molwt>
<charge>0</charge>
<spwt>2e5</spwt>
</material>
```

Each material interaction involves at least three participants: source, target, and product. The distinction between sources and products becomes blurry when dealing with collisions. However, they are clearly distinct when dealing with surface interactions. In this case, the source is the "flying" component. The target is the material that the source hits – the material from which the surface is made of. The product is the material the source turns into after undergoing the impact. In this case, we have told the code to turn O+ ions into O atoms after colliding with Stainless Steel surfaces.

When you look in the materials file, you will see that the specific weight of the oxygen atoms (O), 2e5, differs from the specific weight of the oxygen ions (O+), 5e5. The code takes this into account, and creates, on average, 2.5 atom particles per each impacting ion. You can test this out yourself by changing the value and seeing the number of particles change. The actual density of oxygen atoms will however stay the same, but the data will become noisier as the number of particles is reduced. This can be seen below in Figure 1.
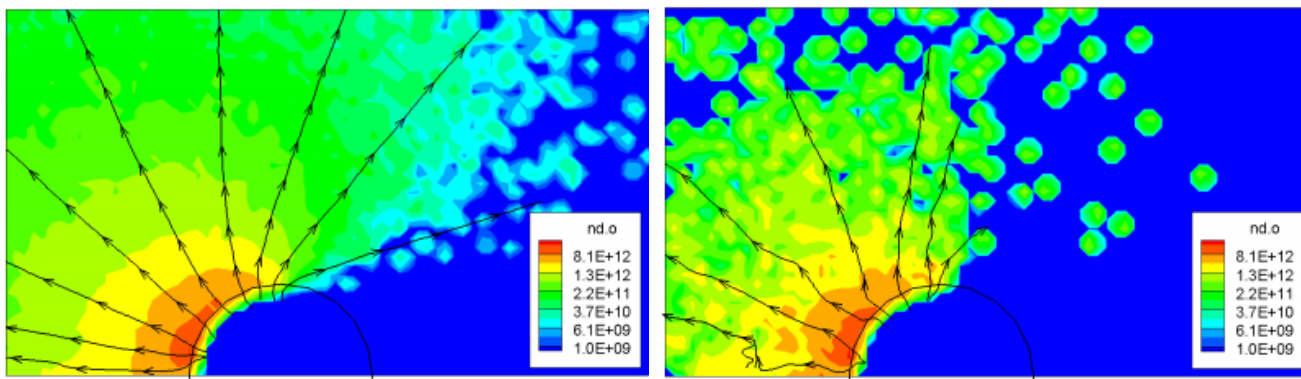
Figure 6. Density of neutrals from surface recombination of impacting ions. Images compare the effect of specific weight on results: 2e5 (left), and 2e7 (right). Instantaneous results.

Material Interaction Model

So far we have only told the code to turn O+ into O. However, we have yet to specify how the new particles will leave the surface. This is done via the model field. Even relatively smooth surface will contain irregularities on the atomic scale. Furthermore, in many cases, incoming molecules do not bounce off the surface like a tennis ball. Instead, they momentarily settle on the surface and then they are re-emitted in a direction that tends to follow Lambert's cosine law. The cosine model models this behavior. The angle of the emitted particle will scale proportionally to the cosine of angle between the velocity vector and the surface normal. Some additional models that are available include specular and diffuse (random) reflection. The c_{rest} and c_{accom} fields control the post impact velocity. The coefficient of restitution, $c_{rest} = v_2/v_1$ is primarily applicable to finite-sized dust particles and for molecular simulations we will usually keep it at 1. The coefficient of thermal accommodation specifies the fraction of incoming particles that will completely forget their

incoming velocity and will instead come off with a velocity corresponding to the thermal velocity of the surface. The overall algorithm is as follows:

```
v2 = v1*c_rest          /*post impact velocity*/
R = random();           /*pick a random number in [0,1)*/
if (R<c_accom)
   v2 = v_th*sampleMaxwellian();

/*create particle with velocity magnitude v2*/
```

Complex Interaction Types
In the above example, all incoming ions turned into neutrals and were re-emitted. However, what if we wanted to model a situation where a fraction of particles stick to the surface, another fraction is reflected specularly, and only the final fraction is emitted according to the cosine law? This is quite easy in Starfish. Starfish allows you to define multiple interaction types with a prescribed probability of occurrence. As an example, let's consider a more complex interactions file:

```
<!-- material interactions file -->
<material_interactions>

<surface_hit source="O+" target="SS">
<product>O</product>
<model>cosine</model>
<prob>0.4</prob>
<c_accom>0.5</c_accom>
<c_rest>0.9</c_rest>
</surface_hit>

<surface_hit source="O+" target="SS">
<product>O</product>
<model>specular</model>
<prob>0.2</prob>
<c_accom>0</c_accom>
<c_rest>1.0</c_rest>
</surface_hit>

</material_interactions>
```

We have now specified two surface_hit fields. In addition, we added a new field called prob. This field gives the probability for each model. As you can see, these two probabilities add up to a value less than 1.0. This is OK, the remaining particles will be handled by default handler, one that absorbs incoming particles.

Step 4: Steady State, Surface Flux, and Data Averaging

We next learn how to export surface properties, such as surface flux and deposition rate. We will also set up averaging to obtain averaged field properties. In the previous step, we added surface recombination of ions into neutrals. The more complex surface model had a fraction of ions stick to the cylinder. Now let's assume that we want to determine the rate with which ions are arriving at the object, and also how much stuff is sticking to it. These are just two examples of surface (boundary) properties that can be exported from the simulation.

But before we start discussing surface flux, we need to introduce the concept of steady state. Many computer simulation methods, especially ones based on kinetic approaches, such as PIC and DSMC, work by integrating simulation particles forward in time from some known initial state. The simulation will initially pass through a transient state in which the results are constantly changing and are not indicative of the final steady solution. As such, we need to wait until steady state to start collection cumulative data. Starfish automatically waits until steady state before starting to collect properties such as surface flux. This is an important point to note if you want to export cumulative data. By default, the steady state is determined automatically. But you can also override it. As an example, here is a time command which instructs the code to assume that steady state is reached at time step 100.

```
<time>
<num_it>500</num_it>
<dt>5e-7</dt>
<steady_state>100</steady_state>
</time>
```

One thing that occurs once steady state is reached is that the code will start collecting information about particles hitting surfaces. This includes properties such as flux of individual materials, as well as the mass deposition rate, corresponding to the particles that stick (are absorbed) to the surface. We can output these properties by adding list of variables to the `output` statement. The result is shown in Figure 7.

```
<output type="boundaries" file_name="boundaries.dat" format="tecplot">
<scalars>flux.o+, flux-normal.o+, depflux.o+, flux, deprate, depflux</scalars>
</output>
```
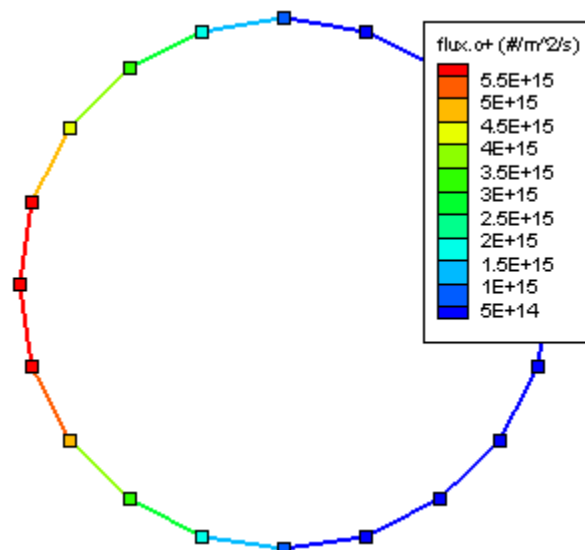

Figure 7. Surface flux saved as surface (boundary) data.

Data Averaging

Since results from kinetic codes are quite noisy, it is a good practice to average results over several time steps to get both smoother plots, and to eliminate outlier data arising from statistical noise. This is done in Starfish with the `averaging` command. The syntax is

```
<!-- setup averaging -->
<averaging frequency="2">
<variables>phi, nd.o+, nd.o</variables>
```

```
</averaging>
```

The averaging starts automatically at steady state, and new data will be added every 2 time steps. The variables lines lists the variables to be averaged. Since averaging data adds a computational overhead, the code averages just the variables that are specified here. These averaged values are then exported using the standard `output` command, with the caveat that the averaged versions will have the base ending in "-ave". For instance,

```
<!-- save results -->
<output type="2D" file_name="field.dat" format="tecplot">
<scalars>phi, phi-ave, rho, nd.o+, nd-ave.o+, u.o+, v.o+, nd.o, nd-ave.o, u.o,
v.o</scalars>
</output>
```

This command will output to a file named "field.dat" the following variables: instantaneous potential, averaged potential, instantaneous ion density, averaged ion density, instantaneous neutral density, and averaged neutral density. Figure 8 below shows the differences.
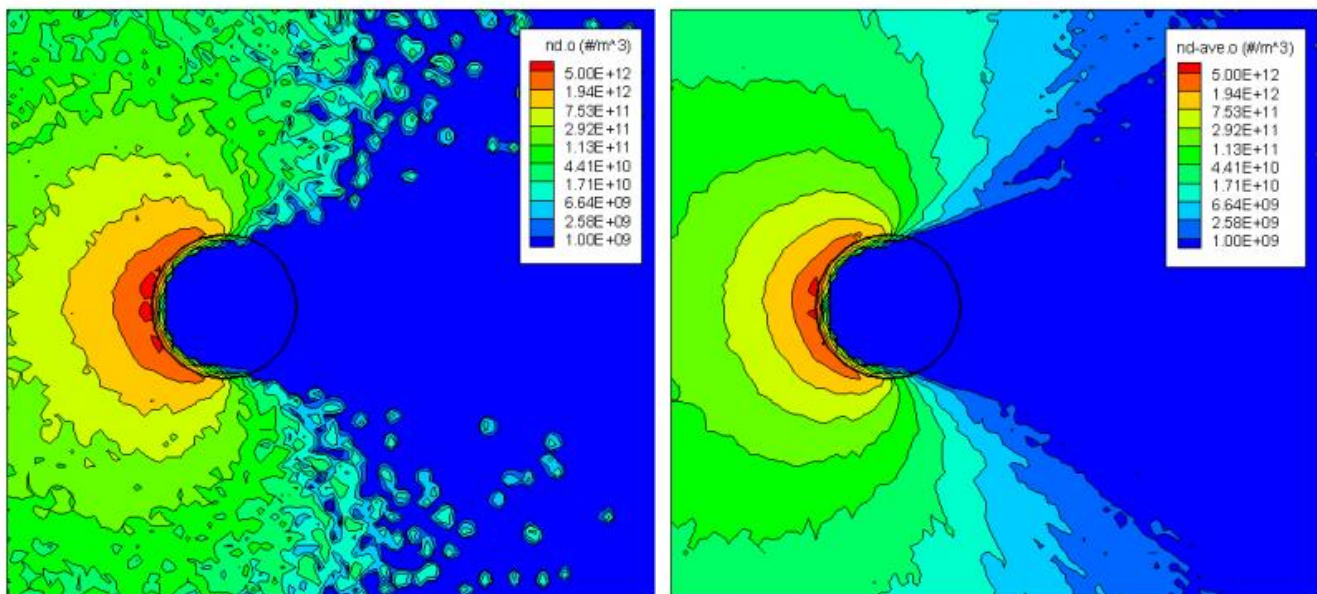
Figure 8. Comparison of instantaneous (left) and averaged (right) neutral densities.

Step 5: MCC Collisions and Chemical Reactions

While previously we discussed the gas/surface interface, we have not yet considered gas interactions. The neutrals and ions currently pass right through without "seeing" each other. Starfish supports three types of material interactions: chemical reactions, MCC, and DSMC. The easiest way to differentiate between these is to think of them as fluid-fluid, particle-fluid, and particle-particle events, respectively. Chemical reactions operate solely with the density and temperature fields and are applicable to models described by a rate equation. They are useful for modeling production or destruction of material in processes such as ionization or recombination.

MCC, or Monte Carlo Collisions, are kinetic-fluid interactions. The source material collides with a target cloud. The number density of the target at the particle position is used to determine the collision probability. If the collision occurs, only the source particle is modified. The target is not affected by the collision. As such, momentum is not conserved. MCC is suitable for cases when the target material is sufficiently more dense than the source, such as when a rarefied ion beam interacts with a dense neutral cloud via the Charge Exchange (CEX) collision. Finally, DSMC (Direct Simulation Monte Carlo) is a

kinetic-kinetic collision process. This method collides particles with other particles in the simulation cell. Both energy and momentum are conserved. This method is suitable for modeling collisions in like gases, such as to model momentum exchange (MEX) collisions in the ion gas. Starfish implements the No Time Counter (NTC) method of Bird [3]. DSMC is the most computationally demanding of these three methods. Material interactions are specified in the *interactions* file which you have already seen before. We used this file previously to add surface recombination. We modify the interactions file as follows:

```
<material_interactions>
...
<!--
<chemistry model="ionization">
<sources>O,e-</sources>
<products>iO+,2*e-</products>
</chemistry>  -->

<mcc model="cex">
<source>O+</source>
<target>O</target>
<sigma>inv</sigma>
<sigma_coeffs>1e-16</sigma_coeffs>
</mcc>

</material_interactions>
```

The chemistry interaction listed here within a comment illustrates how we go about modeling the ionization reaction

$$O + e^- \rightarrow O^+ + 2e^-$$
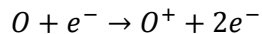
We can write this process as follows:

$$dn_{O^+} = +kn_O n_{e^-} dt$$
$$dn_O = -kn_{O^+} n_{e^-} dt$$

ignoring electron density change. Here "k" is the ionization rate (which is typically function of the electron temperature) and the two "n" correspond to the densities of the atoms and electrons. An example of this interaction is shown in Figure 9. We see that ions are created only in the region containing a neutral population. Additional details about the chemistry model are available online[3].
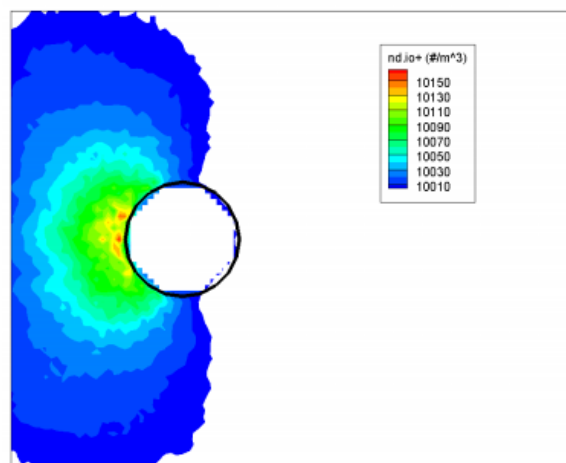

Figure 9. Ions created by the ionization chemistry interaction

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[3] https://www.particleincell.com/2012/starfish-tutorial-part5/

MCC

Let's now move onto MCC. Just as in the case of the chemical reaction, we specify the source and target, as well as the collision model. In this case, we'll be using the CEX handler. This handler models the electron exchange between a fast ion and a slow neutral resulting in a fast neutral and a slow ion,

$$O_{fast}^+ + O_{slow} \rightarrow O_{fast} + O_{slow}^+$$
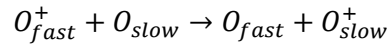
But since this is MCC, we don't actually modify the neutrals. Instead, the neutrals are used to compute the collision probability following $P = 1 - \exp(-n_n g \sigma \Delta t)$, where n_n is the neutral density, g is the relative velocity between the ion and the neutral (with the neutral assumed to be stationary), and σ is the collision cross-section. The sigma model is typically a function of relative velocity, with a number of models existing to describe different collision events. A classic model for modeling CEX is the model of Rapp and Francis. However here, for simplicity, we use a constant cross-section. But even with this relatively large value, collisions are still going to be a very rare event due to the low gas densities. So just to demonstrate this effect, let's go ahead and specify a dense background neutral environment. In the `materials` file, let's modify the oxygen atom by adding an `init` tag,

```
<material name="O" type="kinetic">
<molwt>16</molwt>
<charge>0</charge>
<spwt>2e5</spwt>
<init>nd_back=2e18</init>
</material>
```

This background density will be added to any density from the actual kinetic particles. We can also turn off the potential solver. One way is to replace the Poisson solver with a constant electric field model with zero components,

```
<!-- set zero electric field -->
<solver type="constant-ef">
<comps>0,0</comps>
</solver>
```

This will allow us to see the effect of collisions. The source loads a cold ion beam, and hence, in the absence of forces and collisions, the ions should continue moving in a straight line. Collisions will scatter the motion. You can see this comparison for yourself below in Figure 10. You can see that once the collisions are enabled, we both start seeing diffusion of ions into the wake behind the cylinder, and also the overall density of ions increases. This is due to the presence of many slow ions that are taking a long time to leave the simulation.
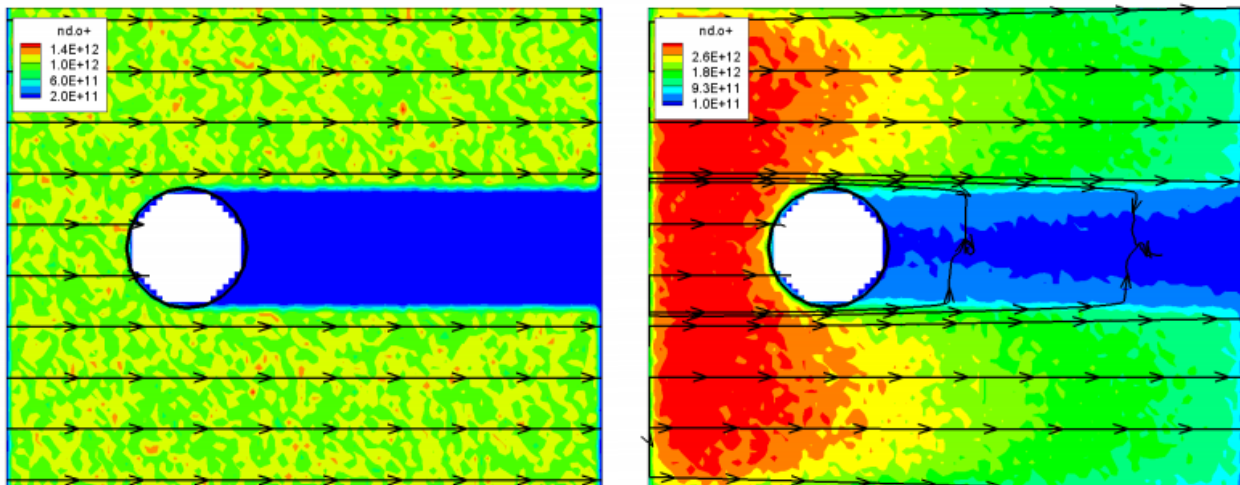

Figure 10. Ion density without (left) and with (right) CEX collisions enabled

III.b) Supersonic expansion of atmospheric gas to vacuum

We now consider a different example motivated by a paper of Jugroot [4]. The authors were interested in simulating nitrogen gas expanding from a 750 Torr (basically atmospheric) environment to a 0.5 Torr tank through a 0.75mm diameter orifice. This is an axisymmetric problem. With the orifice exit plane centered at (0,0), their simulation domain extended to 25 mm in the axial direction and 11 mm in the radial direction. They didn't specify what kind of mesh was used but listed the typical number of cells as 50,000. We set up the problem with a uniform Cartesian mesh with 1e-4 node spacing and 27,500 cells in the low pressure region. To keep the orifice boundary aligned with a mesh edge, the orifice diameter was increased slightly to 0.8mm.
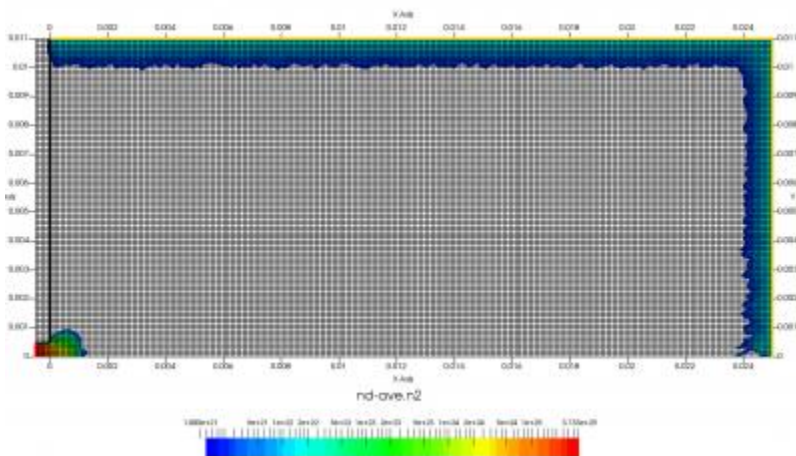
Figure 11. Simulation setup for the supersonic jet expansion example.

The setup for this problem is visualized in Figure 1 above. We will use **ambient** sources to maintain constant pressure along the red and orange boundaries. This source simply creates particles while pressure in the neighboring cell is below some user given threshold. Particles are sampled as thermal gas but can be given optional drift velocity. Besides maintaining pressure, the source can also maintain density. These two properties are related by the ideal gas law, . The black boundary is a solid wall diffusely reflecting incident molecules. Temperature of this wall will be set to the same temperature as the injected gas. Figure 1 shows results after 200 time steps. As you can see, we start with an initially empty domain. I experimented with prefilling the low density region with the 0.5 Torr gas but found it to make no difference.

Input Files

We will now go through the input files needed by the simulation. You will find them in the `tutorial/dsmc/jet` directory. We start with the main `starfish.xml` file. As you can see, it's quite short. We tell the simulation to run for 70,000 time steps, with steady state forced at time step 20,000. This controls when averaging begins. The automatic steady state checking code is not robust, and I wanted to make sure we are truly at steady state when we start collecting data. I also included optional restart code. One other thing you may note is a lack of code specifying averaging. **As of v0.16, velocities, density, and temperature are automatically averaged for kinetic species.**

```
<simulation>
<note>DSMC gas expansion</note>
<log level="Log" />

<!-- load input files -->
<load>domain.xml</load>
<load>materials.xml</load>
<load>boundaries.xml</load>
```

```
<load>interactions.xml</load>
<load>sources.xml</load>

<!-- set time parameters -->
<time>
<num_it>70000</num_it>
<dt>1e-8</dt>
<steady_state>20000</steady_state>
</time>

<!-- run simulation -->
<starfish/>

<!-- save results -->
<output type="2D" file_name="field.vts" format="vtk">
<scalars>nodevol, p, nd-ave.n2, t.n2, t1.n2, t2.n2, t3.n2,  nu, mpc.n2, dsmc-
count</scalars>
<vectors>u-ave.n2, v-ave.n2, w-ave.n2</vectors>
</output>

<output type="boundaries" file_name="boundaries.vtp" format="vtk">
<scalars>flux.n2, flux_normal.n2</scalars>
</output>

</simulation>
```

The variables that we are outputting include node volume, total pressure, average number density of nitrogen, total temperature, temperature components for the three spatial directions, average velocity components, collision rate, average number of macroparticles per cell, and average number of collisions per cell. All this data is saved as point data. In the future, I will make the output algorithm more user friendly by having it save velocity components directly as vectors.

The domain.xml file specifies the uniform mesh used for particle push, collisions, and sampling:

```
<domain type="zr">
<mesh type="uniform" name="mesh">
<origin>-5e-4,0</origin>
<spacing>1.0e-4, 1.0e-4</spacing>
<nodes>256, 111</nodes>
<mesh-bc wall="bottom" type="symmetry"/>
</mesh>
</domain>
```

It is not necessary to specify symmetry on $r = 0$ the edge for an axisymmetric code (domain type="zr") but I left it here in case you want the run the code in the xy mode (domain type="xy")

The materials.xml file lists known materials used for specifying boundaries and gas particles,

```
<materials>

<material name="N2" type="kinetic">
<molwt>28</molwt>
<charge>0</charge>
<spwt>1e11</spwt>
```

```
<ref_temp>275</ref_temp>;
<visc_temp_index>0.74</visc_temp_index>
<vss_alpha>1.00</vss_alpha> <!--1.36-->
<diam>4.17e-10</diam>
</material>

<material name="SS" type="solid">
<molwt>52.3</molwt>
<density>8000</density>
</material>

</materials>
```

The file lists two materials: nitrogen molecules and stainless steel for surfaces. One important thing to note here is that for a kinetic material (flying gas particles) we also specify various DSMC parameters. These values for nitrogen come from Tables A1, A2 and A3 in Appendix A of Bird's 2003 book. The vss_alpha can be used to turn on the Variable Soft Sphere (VSS) collision model. Value of 1 results in the faster Variable Hard Sphere (VHS) being used. I ran few cases and did not observe any significant differences between the two and hence we'll be using VHS in this example. You can speed up the code by using a higher specific weight with the risk of adding numerical error due to not having enough particles per cell.

The boundaries.xml file specifies surface boundaries in an SVG format. You could generate the segments for complex geometries using "path to SVG" in GIMP or Inkscape, but for a simple geometry, you can just make the file by hand,

```
<boundaries>

<boundary name="wall" type="solid">
<material>SS</material>
<path>M 0, 11e-3 L 0,8e-4 -1e-3,8e-4</path>
<temp>288</temp>
</boundary>

<boundary name="inlet" type="solid">
<material>SS</material>
<path>M wall:last L -1e-3,0</path>
<temp>288</temp>
</boundary>

<boundary name="ambient" type="virtual">
<path>M 25e-3,0 L 25e-3,11e-3 0,11e-3</path>
</boundary>

</boundaries>
```

The "ambient" boundary is marked as virtual. This allows this boundary to be used when specifying particle sources but is subsequently invisible to particles during the push. Although "inlet" is marked as solid, it doesn't seem to make a difference. A virtual inlet means that a particle moving back to the tank is removed, and subsequently new particle is generated by the ambient source. However, since both use the same algorithm to sample a half Maxwellian, the result is the same.

Particles sources are listed in the sources.xml file,

```
<sources>

<!--high pressure tank-->
<boundary_source name="inlet_750Torr" type="ambient">
<enforce>pressure</enforce>
<material>N2</material>
<boundary>inlet</boundary>
<drift_velocity>0,0,0</drift_velocity>
<temperature>288</temperature>
<total_pressure>1.0e5</total_pressure>
</boundary_source>

<!--ambient environment-->
<boundary_source name="amb_0.5Torr" type="ambient">
<enforce>pressure</enforce>
<material>N2</material>
<boundary>ambient</boundary>
<drift_velocity>0,0,0</drift_velocity>
<temperature>288.0</temperature>
<total_pressure>66.66</total_pressure>
</boundary_source>

</sources>
```

As you can see, we are specifying two sources of type ambient. This source attempts to maintain constant density, pressure, or partial pressure (as given by the enforce parameter) in cells along the given boundary. Particles are sampled from a half-Maxwellian at the given temperature (288K). The first source generates particles for the 750 Torr reservoir, while the second source generates particles to fill the low pressure tank. Pressures are given in Pascal, hence values in Torr need to be multiplied by 133.322.

Finally, we have interactions.xml file, which specifies particle-surface and particle-particle interactions,

```
<material_interactions>
<surface_hit source="N2" target="SS">
<product>N2</product>
<model>diffuse</model>
<prob>1.0</prob>
</surface_hit>

<dsmc model="elastic">
<pair>N2,N2</pair>
<sigma>Bird463</sigma>
</dsmc>

</material_interactions>
```

This file tells the simulation that a nitrogen molecule hitting a stainless steel surface should reflect diffusely. Collisions between nitrogen molecules are handled with DSMC, with the collision cross-section given by Equation 4.63 in [3].

Results

Once the simulation finishes, you will have a file called `field.vts` which you can visualize using Paraview, Figure 12 The online article discusses some steps for visualizing this file. Figure 13 shows the gas number density, pressure, and temperature. We can clearly see the formation of a the triple point and a Mach disc.
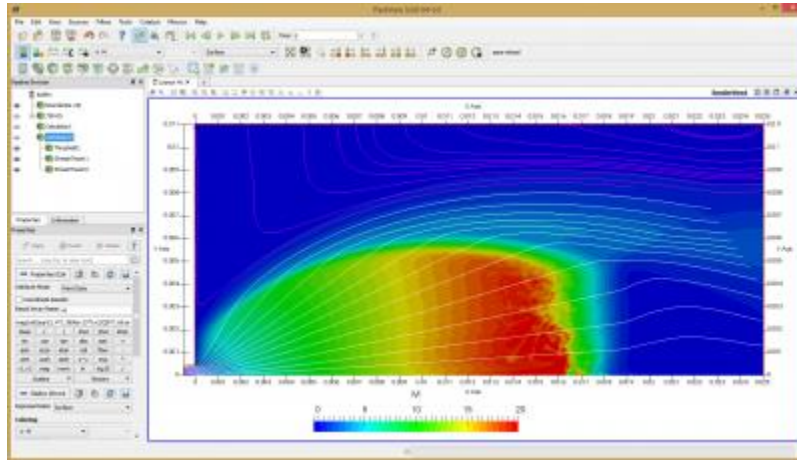
Figure 12. Mach number visualized in Paraview with streamlines added
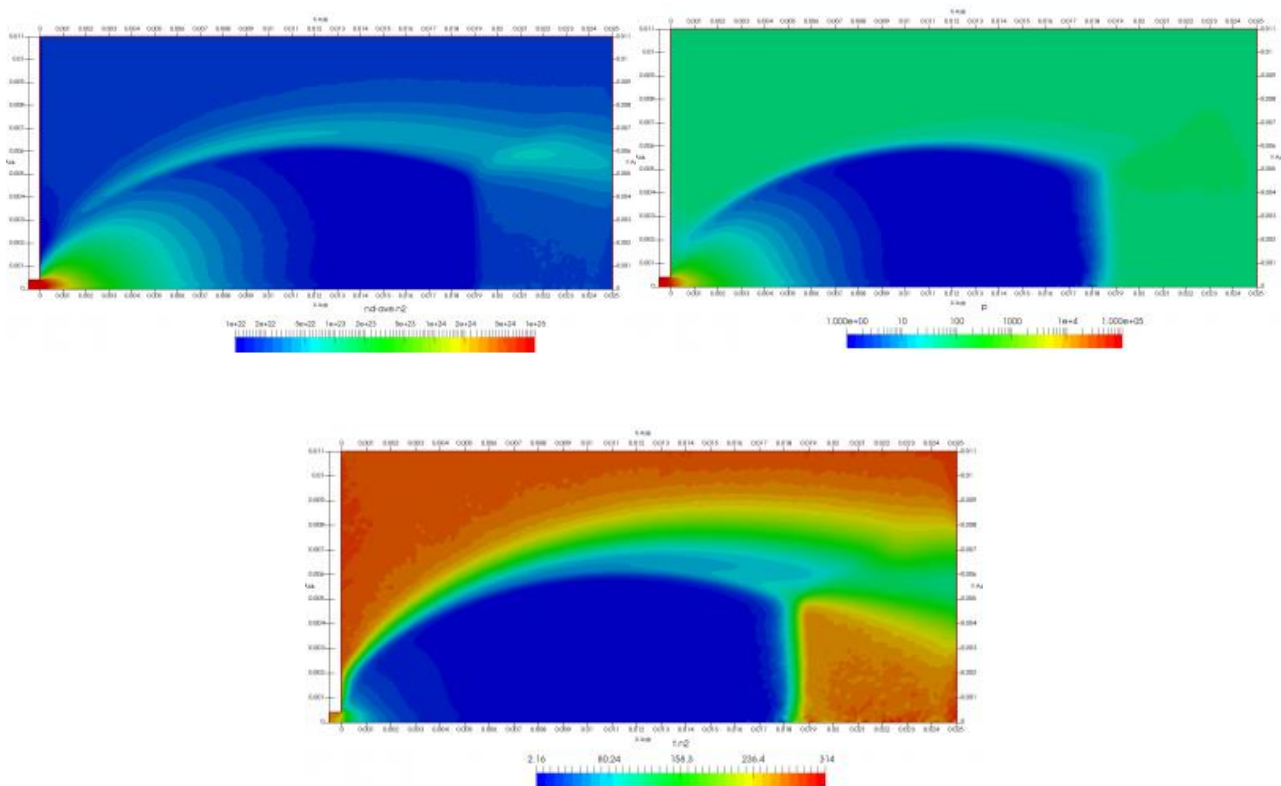
Figure 13. Number density, pressure, and temperature

IV. Extending Starfish-LE

The core Starfish-LE code can be easily extended using plugins. To do so, create a new project inheriting starfish-LE.jar. In your project, define a new main function which initializes an ArrayList of classes inherited from **Plugin**. Then instantiate a new Starfish object and call its start function with this list. This is in fact demonstrated in Starfish-LE default main which uses CollisionsPlugin as a demo.

```
public static void main(String args[])
{
    /*demo of starting Starfish with plugins*/
    ArrayList<Plugin> plugins = new ArrayList<Plugin>();
    plugins.add(new CollisionsPlugin());

    /*make a new instance*/
    new Starfish().start(args, plugins);
}
```

Each command that can be called from the XML input file corresponds to an object derived from **RunnableModule**. The code begins by registering known modules such as "time", "starfish", "output" and so on. Next, the **register** method is called on each provided plugin:

```
/*register modules*/
RegisterModules();

if (plugins!=null)
    for (Plugin plugin:plugins)
        plugin.register();
```

Withing this register method you can add whatever code is needed to extend the code capabilities. For instance, the Collisions plugin registers additional interaction types and a collision cross-section as:

```
public void register()
{
    /*add new interactions*/
    InteractionsModule.registerInteraction("DSMC",DSMC.DSMCFactory);
    InteractionsModule.registerInteraction("MCC", MCC.MCCFactory);

    /*add cross-section*/
    InteractionsModule.registerSigma("Bird463",SigmaPlus.makeSigmaBird463);
}
```

Please do not hesitate to contact us for more specific information.

V. Bugs and Future Work

Please report any bugs or feature requests to info@particleincell.com.

Current work on Starfish includes the following:
1. Re-enabling of multi-mesh support
2. Addition of automatic adaptive mesh refinement
3. Improvements in parallelization by adding support to additional functions
4. Implementation of an electromagnetic EM-PIC model
5. Addition of fluid solver

VI. Command Reference

This section summarizes all commands that can be included in the **starfish.xml** file. Each key can be supplied as an attribute or as an XML node, for instance

<starfish randomize="true"/>

and

<starfish>
<randomize>true</randomize>
</starfish>

are identical. Examples of data field types are given below.

type	description	example(s)
int	integer (whole number) value	-1
int2	two integers separated by comma	41,50
float	a floating point number in double precision	1.06e23
float2	two floats separated by comma	1.07,-3.2
float_list	arbitrary number of comma-separated floats	-23.2,0,12.8
bool	a true or false value	true
string	any text	inlet
string_list	multiple comma separated strings	pressure, nd.xe
string_pairs	multiple comma separated strings in "s1=s2" format. The "s1=" part is not needed if "s2=s2".	bfi=bi, sigma
string_tupples	multiple pairs of strings grouped inside square brackets	[u.xe,v.xe], [efi, efj]
element	a valid child XML element	<output> ... </output>

VI.a) General

VI.a.1) NOTE			
Prints the specified message to the screen and log file.			
Key	**Type**	**Default**	**Description**
N/A	string		Note body
Example			
`<note>Simulation of ion flow past a charged sphere</note>`			

VI.a.2) LOG			
Controls logging level			
Key	**Type**	**Default**	**Description**
level	string		One of [DEBUG, LOG_LOW, LOG, MESSAGE, WARNING, ERROR, EXCEPTION]. Error and exception messages get printed regardless of the log level.
Example			

```
<note>Simulation of ion flow past a charged sphere</note>
```

VI.a.3) RESTART			
Controls saving and reloading of restart data. Currently only particle data are saved. Support for field and fluid materials saving and restarting is pending.			
Key	**Type**	**Default**	**Description**
it_save	bool	500	Frequency of restart data saves
nt_add	int	-1	Number of additional time steps to run after restart load if >0
load	bool	false	Controls whether restart file should be loaded
save	bool	false	Controls whether restart data should be saved
Example			
`<restart it_save="200" nt_add="2500" load="true" save="false" />`			

VI.a.4) STARFISH			
Runs the actual simulation.			
Key	**Type**	**Default**	**Description**
randomize	bool	true	Will randomize the random number generator if true. Set to false to replicate the same simulation.
max_processors	int	num CPUs -1	Maximum number of threads to use for multithreading. By default set to CPU "number of cores" minus 1.
Example			
`<starfish randomize="true" />`			

VI.a.5) STOP			
Stops the simulation. Used for debugging, as the rest of the input file will not processed. Otherwise, the rest of the commands would need to be commented out.			
Key	**Type**	**Default**	**Description**
Example			
`<stop />`			

VI.a.6) TIME			
Controls the duration of the simulation.			
Key	**Type**	**Default**	**Description**
dt	float		Simulation time step, in seconds.
num_it	int		Number of time steps to simulate.
steady_state	string / int	auto	Time step at which the steady state is reached. If "auto", Starfish automatically sets steady state based on differences in particle counts.
Example			
`<time>`			

```
<dt>5e-6</dt>
<num_it>1000</num_it>
</time>
```

VI.b) Input / Output

VI.b.1) ANIMATION			
Wrapper to periodically save simulation results. Works by executing <output> at the specified interval.			
Key	Type	Default	Description
start_it	int		Time step at which output should begin
frequency	int		Number of time steps between file saves
output	element		Entire <output> XML element, following syntax as noted below. For VTK files, file name will be modified to include the time step number.
Example			
<animation start_it="1" frequency="50"> <output type="2D" file_name="results/field_ani.vts" format="vtk"> <scalars>phi, nd.xe+,nd.xe</scalars> <vectors>[efi, efj], [u.xe+,v.xe+]</vectors> </output> </animation>			

VI.b.2) AVERAGING			
Enables averaging of specified variables. The averaged values will have "-ave" append to the prefix. For instance, the average number density of o+ will be called "nd-ave.o+", while "nd.o+" will contain the instantons data. Starting time step should correspond to time after steady state is reached.			
Key	Type	Default	Description
frequency	int	1	Number of time steps between averaging samples
start_it	int	-1	Starting time step for averaging
variables	string_list		List of variables to average
Example			
<averaging frequency="25" start_it="10000"> <variables>phi,rho,nd.o+,nd.e-,u.o+,v.o+</variables> </averaging>			

VI.b.3) LOAD_FIELD			
Loads field data from a file. Can be used, among other things, to load an external magnetic field.			
Key	Type	Default	Description
format	string	TECPLOT	File format. By default, the code supports TECPLOT or TABLE. A TECPLOT file should list variables on a single VARIABLES line. The TABLE format is assumed to start with ni,nj, and is hardcoded for "z,r,B,Bz,Br" data.
file_name	string		name of the file to load

coords	string_list		names of two file variables to correspond to XY, RZ, or ZR, according to the specified <domain> type.
vars	string_pairs		variables to load in "starfish_var=file_var" format. The assignment part is not needed if the file variable is the same as the expected Starfish variable name.

Example

<pre><load_field format="tecplot" name="bfield">
<file_name>bfield.dat</file_name>
<coords>z,r</coords>
<vars>bfi=bz,bfj=br,lambda</vars>
</load_field>
 	
-- example of a Tecplot file format --
VARIABLES = "z", "r", "n_n"
ZONE I=52, J=18, F=POINT
0.0491 0.0071 1.09994e+014
 	
-- example of a Table format --
47 22
  -0.018 0   0.03   0.03   0</pre>

VI.b.4) OUTPUT			
Wrapper to periodically save simulation results. Works by executing <output> at the specified interval.			
Key	**Type**	**Default**	**Description**
type	string		Type of output to generate. Must be one of "1D", "2D", "boundaries", or "particles".
file_name	string		Name of output file
format	string		Output file format. Currently only "TECPLOT" and "VTK" are supported.
scalars *(or variables)*	string_list		List of node-centered scalar variables to output. For backward compatibility, "variables" can be used as well.
cell_data	string_list		List of cell-centered scalars to output
vectors	string_tupples		Pairs of node-centered scalar variables to group together as vectors. Only affects VTK output.
TYPE = "1D"			
Saves a slice of mesh data by exporting data only along a single given "i" or "j" index.			
mesh	string		Name of the mesh to output (only a single mesh output is supported).
index	string		Logical grid position to output in format "I=xx" or "J=xx"
TYPE = "2D"			
Saves mesh field data. No additional inputs.			
TYPE = "BOUNDARIES"			

Saves surface data along boundaries. No additional inputs.			
TYPE = "PARTICLES"			
Exports user specified number of randomly selected particles.			
count	int		Number of particles to output
Example			

```
<output type="1D" file_name="profile.vts" format="vtk">
<mesh>mesh1</mesh>
<index>I=1</index>
<variables>phi, rho, nd.xe+</variables>
</output>

<output type="2D" file_name="results/field.vts" format="vtk">
<scalars>psi, phi, te, rho, sigma, nd.xe+</scalars>
<vectors>[ue,ve], [u.xe+, v.xe+], [efi, efj], [jx,jy]</vectors>
</output>

<output type="boundaries" file_name="boundaries.vtp" format="vtk">
<variables>deprate.xe+, flux-normal.xe+</variables>
</output>

<output type="particles" file_name="particles.dat" format="tecplot">
<species>ti2+,e-</species>
<count>10000,10000</count>
</output>
```

VI.b.5) PARTICLE_TRACE			
Command to sample position and velocity of a specified particle to generate a trace file			
Key	**Type**	**Default**	**Description**
file_name	string		Name of output file
format	string	TECPLOT	File format, currently only "TECPLOT" and "VTK" are supported.
material	string		Material of the sampled particle
id	int		Particle id
start_it	int		Starting time step for output
Example			

```
<particle_trace file_name="trace.dat" material="HC">
<id>20685</id>
<start_it>495</start_it>
</particle_trace>
```

VI.b.6) STATS			
Command to control frequency of saves to a global diagnostics file			
Key	**Type**	**Default**	**Description**

file_name	string	starfish_stats.csv	Stats file name
skip	int	1	Output frequency. Value <=0 disables file output.
Example			
`<stats skip="10" />`			

VI.c) Materials

VI.c.1) MATERIALS			
Definition of materials known to the simulation. Contains one or more <material> elements.			
Key	**Type**	**Default**	**Description**
material	element		Material definition. See the following entry for Material for data fields.
Example			

`<materials>`
 	
`<material name="Ar" type="kinetic">`
`..`
`</material>`
 	
`<material name="SS" type="solid">`
`..`
`</material>`
 	
`</materials>`			

VI.c.2) MATERIAL			
Definition of a single material embedded within <materials> element			
Key	**Type**	**Default**	**Description**
type	string		Material type. Can be one of "solid" (materials that do not change), "kinetic" (materials simulated with particles), and "fluid_diffusion" (density updated with advection-diffusion solver). Additional material types can be provided by plugins.
name	string		name of the material
init	string_list		List of one or more initial values for the following fields: "nd", "nd_back" (#/m^3), "u", "v" (m/s), and "T" (K). With the exception of nd_back, these entries are currently used only to set the initial values of density, velocity, or temperature on the computational mesh. The value of nd_back is added to the density computed from particles and can be used to set a minimum material density floor.
type = "SOLID"			
molwt	float		material molecular weight
type = "KINETIC"			
molwt	float		material molecular weight

charge	float		material charge in elementary charge units
spwt	float		default specific weight, number of real molecules pre simulation particle
frozen	bool	false	particle positions and velocities will not update if set to true. Typically used to freeze particles from a restart file to create a fixed background.
ref_temp	float	275	reference temperature for DSMC cross-section model
visc_temp_index	float	0.85	viscosity index for DSMC model
vss_alpha	float	1	VSS coefficient, VHS logic used if 1
diam	float	5e-10	molecular diameter in m
type = "FLUID_DIFFUSION"			
molwt	float		material molecular weight
charge	float		material charge in elementary charge units
mu	float		material dynamic viscosity in kg/m/s
Example			

```
<!-- charged particle with fixed background floor -->
<material name="Xe+" type="kinetic">
<molwt>131.3</molwt>
<charge>1</charge>
<init>nd=1e15,nd_back=1e4,T=1000 </init>
<mu>0</mu>
<spwt>2e9</spwt>
</material>

<!-- neutral kinetic material with DSMC data -->
<material name="Ar" type="kinetic">
<molwt>39.94</molwt>
<charge>0</charge>
<spwt>5e11</spwt>
<ref_temp>273</ref_temp>;
<visc_temp_index>0.81</visc_temp_index>
<vss_alpha>1.00</vss_alpha>
<diam>4.17e-10</diam>
</material>

<!-- solid material -->
<material name="SS" type="solid">
<molwt>52.3</molwt>
</material>
```

VI.d) Material Interactions

VI.d.1) MATERIAL_INTERACTIONS			

Controls inter-material interactions, including the gas material / surface boundary interface. Interactions are specified via child elements. Starfish natively supports four types of interactions:
   1. surface_hit: interaction between material and a surface boundary
   2. dsmc: interaction between two kinetic materials
   3. mcc: interaction between a kinetic source and a fluid target
   4. chemistry: interaction between two fluid materials			

Key	**Type**	**Default**	**Description**
surface_hit / mcc / chemistry / dsmc	element		Available interaction types. Additional types can be implemented by plugins.
Example			
<pre><material_interactions>\n\n<surface_hit>\n...\n</surface_hit>\n\n<dsmc>\n...\n</dsmc>\n\n</material_interactions></pre>			

VI.d.2) SURFACE_HIT			
Command to control frequency of saves to a global diagnostics file			
Key	**Type**	**Default**	**Description**
file_name	string	starfish_stats.csv	Stats file name
skip	int	1	Output frequency. Value <=0 disables file output.
Example			
<stats skip="10" />			

VI.d.3) DSMC			
Enables DSMC collisions between two kinetic materials			
Key	**Type**	**Default**	**Description**
pair	string_list		Names of the two materials participating in this interaction
model	string		Currently only "elastic" is supported
frequency	int	1	
sig_cr_max	float	1e-16	
sigma	string		Collision cross-section. Natively the following models are supported:

			• const: $\sigma = c_0$ • inv: $\sigma = c_0/g$ • bird463: $\sigma = 0.25\pi d_{ref}^2 \left(\frac{2kT_{ref}}{m_r g^2}\right)^{\omega-0.5} /\Gamma(2.5-\omega)$, equation 4.63 in Bird 2003
sigma_coeffs	float_list		Collision cross-section coefficients

Example

```
<dsmc model="elastic">
<pair>N2,N2</pair>
<sigma>Bird463</sigma>
</dsmc>
```

VI.d.4) MCC

Enables MCC collisions between a kinetic and fluid / kinetic target. Properties of the target material are not affected by the collision and hence this interaction is suitable only for cases of a rarefied source material interacting with a much denser target. A kinetic material can be used as the target, in which case, the density obtained by scattering particles to the grid will be used to obtain collision probability.

Key	Type	Default	Description
source	string		Name of the source kinetic material.
target	string		Name of the target fluid or kinetic material
product		<source>	Optional post-collision material of the source. By default, there is no species change.
model			Collsion model. Can be "MEX" / "ELASTIC" for momentum transfer, or "CEX" for charge exchange collision
sigma	string		Collision cross-section. See description of DSMC for details.
sigma_coeffs	float_list		Collision cross-section coefficients.

Example

```
<mcc model="cex">
<target>ar</target>
<source>ar+</source>
<sigma>inv</sigma>
<sigma_coeffs>1e-16</sigma_coeffs>
</mcc>
```

VI.d.5) CHEMISTRY

Enables fluid-fluid interactions. Densities of source materials (which can be kinetic or fluid) along with temperature (or energy) of a dependent material are used to compute the reaction, $n_{s1}n_{s2}k(T_d)$. Products are then generated accordingly and source material densities are depleted.

Key	Type	Default	Description
sources	string_list		List of reactants with optional multipliers
products	string_list		List of products

rate	element		Reaction rate equation type
RATE			
type	string		Currently only "POLYNOMIAL" is supported. This evaluates $(c_0 + c_1 v + c_2 v^2 + \cdots)c_{mult}$
coeffs	float_list		List of model coefficients
multiplier	float		Coefficient multiplier
dep_var	element		Information about the dependent variable v in the rate model.
DEP_VAR			
mat	string		name of the dependent variable
wrapper	string	NONE	Options are NONE, LOG10, or LOG10ENERGY
Example			

```
<chemistry>
<sources>Xe,e-</sources>
<products>Xe+,2*e-</products>
<rate type="polynomial">
<coeffs>-0.57, 6.1978, -23.19, 30.439, 2.8407, -18.722</coeffs>
<multiplier>1e-20</multiplier>
<dep_var wrapper="log10energy" mat="e-" />
</rate>
</chemistry>
```

VI.e) Boundaries

VI.e.1) BOUNDARIES			
This command is used to define the surface geometry. It contains several <boundary> elements each specifying a particular surface spline.			
Key	**Type**	**Default**	**Description**
boundary	element		Definition of a single boundary
transform	element		Optional, defines global transformation applied to all boundaries
TRANSFORM			
scaling	float2	1,1	Scaling in the i and j direction
translation	float2	0,0	translation in the I and j direction
rotation	float	0	Rotation about the z axis
reverse	bool	false	Flips normal vector orientation
Example			

```
<boundaries>
<transform>
<scaling>1e-3,-1e-3</scaling>
<translation>0,0</translation>
<reverse>true</reverse>
</transform>
```

```
<boundary>...</boundary>
<boundary>...</boundary>
</boundaries>
```

VI.e.2) BOUNDARY			
Defines a single surface boundary spline.			
Key	**Type**	**Default**	**Description**
name	string		Name of the boundary
type	string	solid	Boundary type. Can be one of: SOLID for a solid surface with fixed Dirchlet b.c., OPEN for Neumann b.c. (not fully supported), SYMMETRY for symmetric boundary reflecting particles, VIRTUAL for boundaries useful for attaching sources but that are not affect material propagation, and SINK for an absorbing boundary. Note that some of these are either extraneous or not yet fully implemented.
value	float	0	Boundary condition value. For SOLID boundaries this sets the Dirichlet potential for the Poisson solver.
material	string		Boundary material, only required for SOLID
temp	float	273.15	Boundary temperature, used to compute post-impact velocity
path	string		Spline definition in SVG-like format. The general syntax is [COMMAND] x1,y1 x2,y2 … [COMMAND] x,y. The following commands are supported: "M x,y" move to (x,y), "m dx,dy" move by offset (dx,dy), "L x,y" line to (x,y) from the previous point, "l dx,dy" line to point offset by (dx,dy) from the last point, "C x1,y1 x2,y2,…" smooth cubic spline through points (x1,y1), (x2,y2), … Commands do not need to be repeated, for instance "M x1,y1 L x2,y2 L x3,y3 L x4,y4" can be written as "M x1,y1 L x2,y2 x3,y3 x4,y4". Points need to be specified in counter-clockwise order around an solid boundary (or in clockwise order around an open boundary), as point ordering controls the normal vector orientation. Note that unlike in SVG, cubic splines are specified by simply listing the points through which the spline will pass and the control knot points are omitted.
transform	element		Optional transformation parameters
reverse	bool		Optional, flips normal vector orientation, overridden by entry in <transform> if both defined.
Example			

```
<boundary name="inlet" value="300">
<material>SS</material>
<path>M 0,0 L 400,71</path>
<material>vent</material>
<reverse>true</reverse>
<transform>
<scaling>1e-3,1e-3</scaling>
</transform>
</boundary>
```

```
<boundary name="downstream" type="open">
<path>M inlet:last C 0.086,0.007 0.085,0.014 0.0791,0.02</path>
</boundary>
```

VI.f)   Domain

VI.f.1) DOMAIN			
Specifies details of the computational domain (simulation mesh). Contains one or more <mesh> elements.			
Key	**Type**	**Default**	**Description**
type	string	XY	Controls the meaning of "i" and "j" indexes. Available options are XY, RZ, and ZR. Axisymmetric corrections are applied for RZ and ZR types.
mesh	element		Mesh definition. Currently support for multiple meshes is limited but will be corrected in an upcoming version.
Example			

<pre><!-- domain file -->
<domain type="rz">
 	
<mesh>...</mesh>
<mesh>...</mesh>
</domain></pre>			

VI.f.2) MESH			
Specifies details of a single mesh. Currently two types are supported: uniform Cartesian mesh or an elliptic, body fitted, mesh.			
Key	**Type**	**Default**	**Description**
name	string		Mesh name
type	string		Mesh type, one of UNIFORM or ELLIPTIC
mesh-bc	element		Specifies mesh boundary conditions
type="UNIFORM"			
The following inputs are required for UNIFORM mesh			
origin	float2		Coordinates of i=0,j=0 point
spacing	float2		Distance between nodes
nodes	int2		Number of nodes in i and j direction
type="ELLIPTIC"			
The following inputs are required for ELLIPTIC mesh. This option creates a stretched mesh between four boundaries with a prescribed number of nodes in the i and j direction.			
left	string		Name of the <boundary> forming the left edge
right	string		Name of the boundary for the right edge
bottom	string		Name of the boundary for the bottom edge
top	string		Name of the boundary for the top edge

nodes	int2		Number of nodes in i and j direction
MESH-BC			
value	float	0	Boundary condition value. Currently only used to set Dirichlet boundaries.
wall	string		Mesh wall to apply this boundary to. One of "left", "right", "bottom", or "top".
type	string		Mesh boundary type, supported values include OPEN, DIRICHLET< NEUMANN, PERIODIC, SYMMETRY, SINK, and CIRCUIT.
Example			

```
<mesh type="uniform" name="mesh">
<origin>0, 0</origin>
<spacing>5e-5, 1e-4</spacing>
<nodes>51, 361</nodes>
<mesh-bc wall="left" type="symmetry" />
<mesh-bc wall="bottom" type="neumann" />
</mesh>

<mesh type="elliptic" name="downstream">
<left>exit_plane</left>
<bottom>symmetry_outside</bottom>
<right>downstream</right>
<top>body</top>
<nodes>35,13</nodes>
</mesh>
```

VI.g) Sources

VI.g.1) SOURCES			
Specifies material sources. Starfish supports two types of sources: boundary sources that inject mass along a specified boundary, and volume source that generate mass within the computational mesh.			
Key	**Type**	**Default**	**Description**
boundary_source / material_source / volume_source	element		The actual source definitions
Example			

```
<sources>
<boundary_source>...</boundary_source>
<volume_source>...</volume_source>
</sources>
```

VI.g.2)   BOUNDARY_SOURCE
Specifies material sources. Starfish supports three types of sources: boundary that inject mass along a specified boundary, material sources that act like boundary sources but are applied to all boundaries with the given material, and volume source that generate mass within the computational mesh.

Key	Type	Default	Description
name	string		source name
type	string		source type, one of UNIFORM, MAXWELLIAN, AMBIENT, and COSINE
material	string		name of the injected material
boundary	string		surface boundary name to attach the source to
type="UNIFORM"			
This source injects a cold beam. It is a streamlined implementation of a Maxwellian source with T=0K.			
mdot	float		Mass flow rate in kg/s
v_drift	float		Drift velocity in m/s
type="MAXWELIAN"			
Source for injecting mass sampled from the drifting Maxwellian velocity distribution function			
mdot	float		Mass flow rate in kg/s
v_drift	float		Drift velocity in m/s
temperature	float		Temperature in K
start_it	float	0	Time step to begin injection
end_it	float	-1	Time step to end injection, or -1 to ignore
type="AMBIENT"			
Generates mass in cells adjacent to the specified boundary such that prescribed density or pressure is maintained. Particle velocities are sampled from the Maxwellian distribution.			
drift_velocity	float3	0,0,0	Drift velocity to apply to sampled material
temperature	float		Assumed gas temperature in K, controls injection velocity and also used to scale pressure to density from $P = nkT$.
enforce	string	TOTAL_PRESSURE	Controls which property the source should maintain. Available options are TOTAL_PRESSURE, PARTIAL_PRESSURE, and DENSITY
density	float		Required for enforce="DENSITY", controls the desired number density in m^{-3}.
total_pressure	float		Required for enforce="TOTAL_PRESSURE" or "PARTIAL_PRESSURE", in Pa
partial_pressure	float		Required for enforce="PARTIAL_PRESSURE", used to control the desired species fraction per P_i/P_{tot}
type="COSINE"			
Injects particles with velocity sampled from the cosine distribution about the surface normal			
mdot	float		Injection mass flow rate in kg/s
v_drift	float		Drift velocity in m/s
Example			

`<boundary_source name="neutral_source" type="maxwellian">`
`<material>xe</material>`
`<boundary>inlet</boundary>`			

```
<mdot>4e-7</mdot>
<v_drift>1000</v_drift>
<temp>1000</temp>
</boundary_source>


<boundary_source name="amb_0.5Torr" type="ambient">
<enforce>pressure</enforce>
<material>N2</material>
<boundary>ambient</boundary>
<drift_velocity>0,0,0</drift_velocity>
<temperature>288.0</temperature>
<total_pressure>66.66</total_pressure>
</boundary_source>
```

VI.h) Solver

VI.h.1) SOLVER			
Activates a field solver. Currently only plasma potential solvers are implemented.			
Key	**Type**	**Default**	**Description**
type	string		Solver type
initial_only	bool	false	If set to true, only the initial field will be computed
max_it	float	5000	Maximum number of solver iterations
tol	float	1e-6	Solver tolerance
nl_max_it	float	50	Maximum number of solver iterations for a non-linear solver
nl_tol	float	1e-4	Non-linear solver tolerance
type="CONSTANT-EF"			
This "solver" fixes electric field components to the prescribed value			
comps	float2		Values for Ei, Ej in V/m
type="QN"			
Sets potential from the quasi-neutral Boltzmann relationship $\phi = \phi_0 + kT_{e,0} \ln(n/n_0)$.			
n0	float		Reference number density, #/m^3
Te0	float		Reference temperature in eV
phi0	float		Reference potential in V
type="POISSON"			
Solves the Poisson's equation $\epsilon_0 \nabla^2 \phi = -e(n_i - n_e)$, where n_e is obtained directly from simulation electrons in a linear mode, or is set to $n_e = n_0 \exp\left(\frac{\phi - \phi_0}{kT_{e,0}}\right)$ in the non-linear mode.			
linear	bool	false	Controls how the electron density term is computed.
n0	float	1e15	Reference density for the non-linear term in #/m^3
Te0	float	1	Reference temperature for the non-linear term in eV
phi0	float	0	Reference potential for the non-linear term in V
Example			

```
<!-- non-linear poisson solver example -->
<solver type="poisson">
<n0>1e12</n0>
<Te0>1.5</Te0>
<phi0>0</phi0>
<max_it>100000</max_it>
<tol>1e-3</tol>
<nl_tol>1e-2</nl_tol>
</solver>

<!-- prescribed electric field example -->
<solver type="constant-ef">
<comps>0,0</comps>
</solver>

<!-- quasineutral Boltzmann inversion example -->
<solver type="qn">
<n0>1e12</n0>
<Te0>1.5</Te0>
<phi0>0</phi0>
</solver>
```

VII.   Data Fields

The below table summarizes data field and boundary variables in the baseline configuration. All material-specific fields follow syntax "base.mat", for instance "nd.xe" is the number density of material "xe". Averaged fields generated by the <averaging> command will have "-ave" appended to the base, for instance "phi-ave" and "nd-ave.xe".

VII.a) Mesh Data

Name	Units	Description
VII.a.1) General		
nodevol	m^{-3}	Mesh node volume, used for computing number density
phi	V	plasma potential
rho	C/m^3	charge density
efi,efj	V/m	electric field components
bfi,bfj	T	magnetic field components
p	Pa	total pressure
VII.a.2) Material-Specific (base.mat)		
nd	#/m^3	material number density
u,v,w	m/s	node-averaged gas mean velocity
nd-ave	#/m^3	steady-state averaged number density

u-ave,v-ave,w-ave	m/s	steady-state averaged gas mean velocity
t	K	average gas temperature
p	Pa	gas pressure, obtained from the ideal gas law
t1,t2,t3	K	gas temperature in i,j,k direction
mpc	#	number of simulation macroparticles per cell
count-sum	#	internal variable used to obtain density, contains specific weight sum
u-sum,v-sum,w-sum	m/s	internal variable used to obtain velocity, contains sum of $w_{sp}u$
uu-sum,vv-sum,ww-sum		internal variable used to obtain temperature, contains sum of $w_{sp}u^2$
mpc-sum	#	internal variable used to obtain mpc, contains sum of macroparticles
VII.a.3) MCC		
mcc-count, mcc-count2, …	#	Number of collisions
mcc-nu, mcc-nu2, …	#/s	Collision rate
mcc-real-sum, mcc-real-sum2, …	#	Internal variable used to compute MCC collision count, stores cumulative number of real particles undergoing collisions
mcc-count-sum, mcc-count-sum2, …	#	Internal variable used to compute MCC collision count, stores cumulative number of MCC collisions
VII.a.4) DSMC		
dsmc-count, dsmc-count2, …	#	Number of collisions
nu, nu2	#/s	Collision rate
dsmc-real-sum, dsmc-real-sum2, …	#	Internal variable used to compute DSMC collision count, stores cumulative number of real particles undergoing collisions
dsmc-count-sum, dsmc-count-sum2, …	#	Internal variable used to compute DSMC collision count, stores cumulative number of MCC collisions

VII.b) Boundary Data

Name	Units	Description
VII.b.1) Material-Specific		
flux	#/m²/s	Total number of particles hitting the boundary per second, scaled by boundary area
flux-normal	#/m²/s	Particle flux multiplied by the cosine angle between the incoming velocity vector and surface normal
deprate	kg/s	Rate of mass depositing to the surface
depflux	kg/m²/s	Deposition rate scaled by the boundary area

VIII.   References

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[4] M. Jugroot, C. Groth, T. B, B. V and B. Collings, " Numerical investigation of interface region flows in mass spectrometers: neutral gas transport," *J. of Phys., D: Applied Physics,* vol. 37, pp. 1289-1300, 2004.