# Ion Trajectory Calculation Lab

## Introduction

These labs are designed to demonstrate the impact of the ion trajectory quality parameter on the accuracy of ion trajectories.

**Location: C:\Advance SIMION Class\03. Trajectories and Instances\Trajectory Lab**

## DC Reflection Field Experiment

The first experiment uses linear gradient fields and an ideal grid to test the conservation of energy in linear fields with discontinuities. The fields form an electrostatic trough that acts to reflect the ion into wave-like motions.

### Preparation

Load the reflections.pa# file and refine it to 1.0e-7
Remove all arrays
Load the reflections.iob file into view
Click the Fly'm buttons

### Discussion

The pa with its central ideal mirror forms a reflection trough. Ions are launched with a small amount of kinetic energy in the x direction half way up one side of the trough in y. The ion forms a trajectory wave as it swings across the center grid. Energy is conserved if successive peak heights remain the same (successive ymaxes remain the same).

Note: Two red neutrals are flown to serve as a reference for peak height measurements for the tests described below.

### Experiment

As a test, vary the trajectory quality to 103 or above. Now try 0 and various negative numbers. Notice that 0 or negative numbers do not conserve energy very well. Turn on data recording so that a marker is generated each time step. Notice that time steps bunch near velocity reversals and around the ideal grid discontinuity when trajectory quality is positive. This helps to better conserve the ion's energy in the calculation.

## Second and Third Experiments

These tests uses a RF linear gradient fields between two plates to test the conservation of energy in linear RF fields with discontinuities. The RF field forms an electrostatic RF trough that acts to reflect the ion into wave-like motions.

## RF Mirror Experiment

A sine wave RF is used between the two plates (in y). A collection of ions are given a small ke in x relatively close to one of the plates. Each ion follows a wave-like trajectory.

### Preparation

Load RF Mirror.pa# and refine to 1.0e-7
Remove all PAs
Load RF Mirror.iob into View
Click the Fly'm button

### Discussion

The ions are flown 1/2 cycle (by default) and then killed. The expected peak to peak dy (in mm) using a formal integration of the expected forces is compared to the dy obtained from the simulation.

If you want the ions to keep on flying set the adjustable variable:
Long_Simulation_if_1 to the value of 1.

### Experiment

Note that higher values of trajectory quality improve the higher mass dy accuracies. The issue here is that these ions have small wave sizes in relation to array grid intervals. To improve accuracy you need to either use a higher density array or turn up the trajectory quality to shrink the timesteps in trajectory curvature areas.

## RF Square Wave Experiment

A square wave RF is used between the two plates (in y). A collection of ions are given a small ke in x relatively close to one of the plates. Each ion follows a wave-like trajectory. The square wave will induce conservation of energy problems unless the switch edge can be detected accurately and automatically.

### Preparation

Load RF Square Wave.pa# and refine to 1.0e-7
Remove all Pas
Load RF Square Wave.iob into View
Click the Fly'm button

**Discussion**

The ions are flown 1/2 cycle (by default) and then killed. The expected peak to peak dy (in mm) using a formal integration of the expected forces is compared to the dy obtained from the simulation.

If you want the ions to keep on flying set the adjustable variable:
Long_Simulation_if_1 to the value of 1.

**Experiment**

Note that 0 or negative value of trajectory quality cause considerable errors because of their fixed time step nature.

Note that higher values of trajectory quality improve the higher mass dy accuracies. The issue here is that these ions have small wave sizes in relation to array grid intervals. To improve accuracy you need to either use a higher density array or turn up the trajectory quality to shrink the timesteps in trajectory curvature areas.

Turn on data recording at each time step to verify that SIMION is indeed catching the edge of the RF square wave.