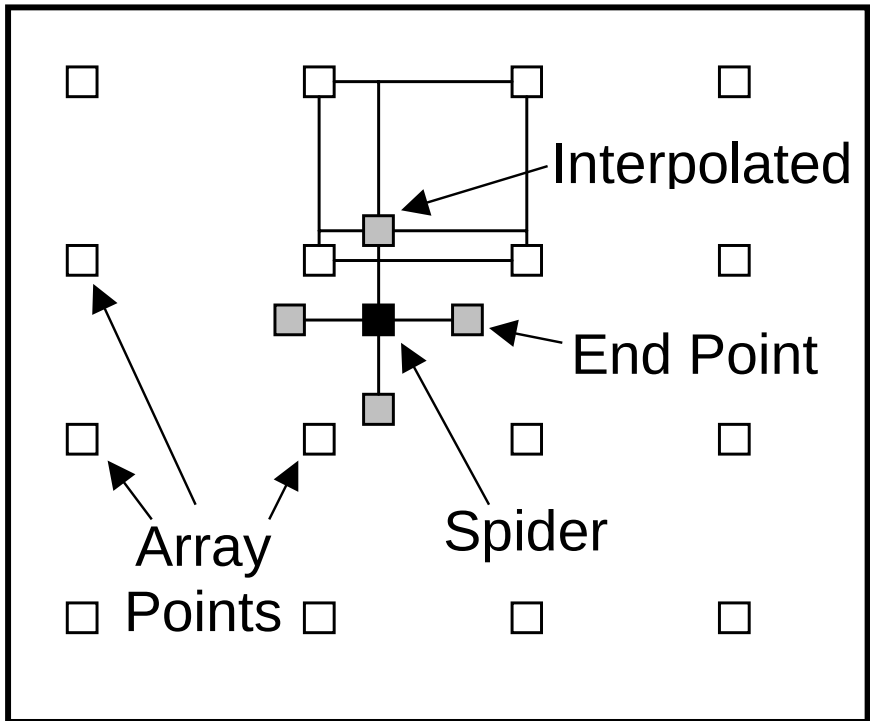
3.a Ion Trajectories

- How field gradients are obtained
- Constant distance step integration
- Stop length step shortening
- Binary boundary approach method
- CV of acceleration provides some vision
- How Trajectory Quality param. controls all
- Flying ions singly or in groups

Obtaining Field Gradients

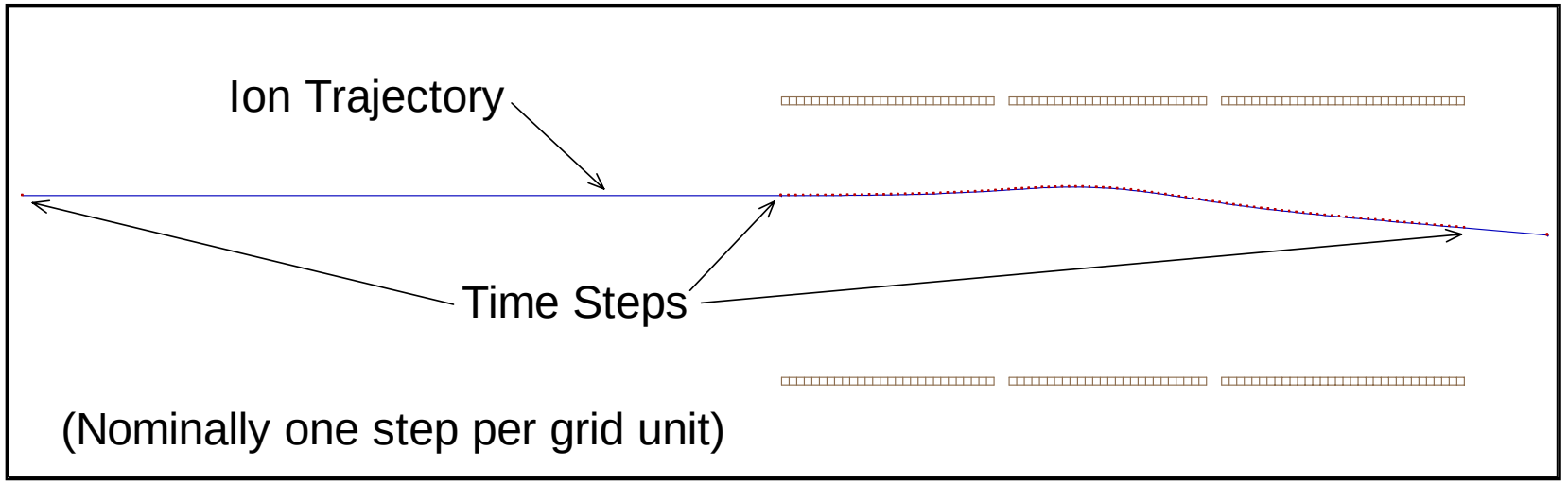
- From Arrays:



- Other: From User Programs

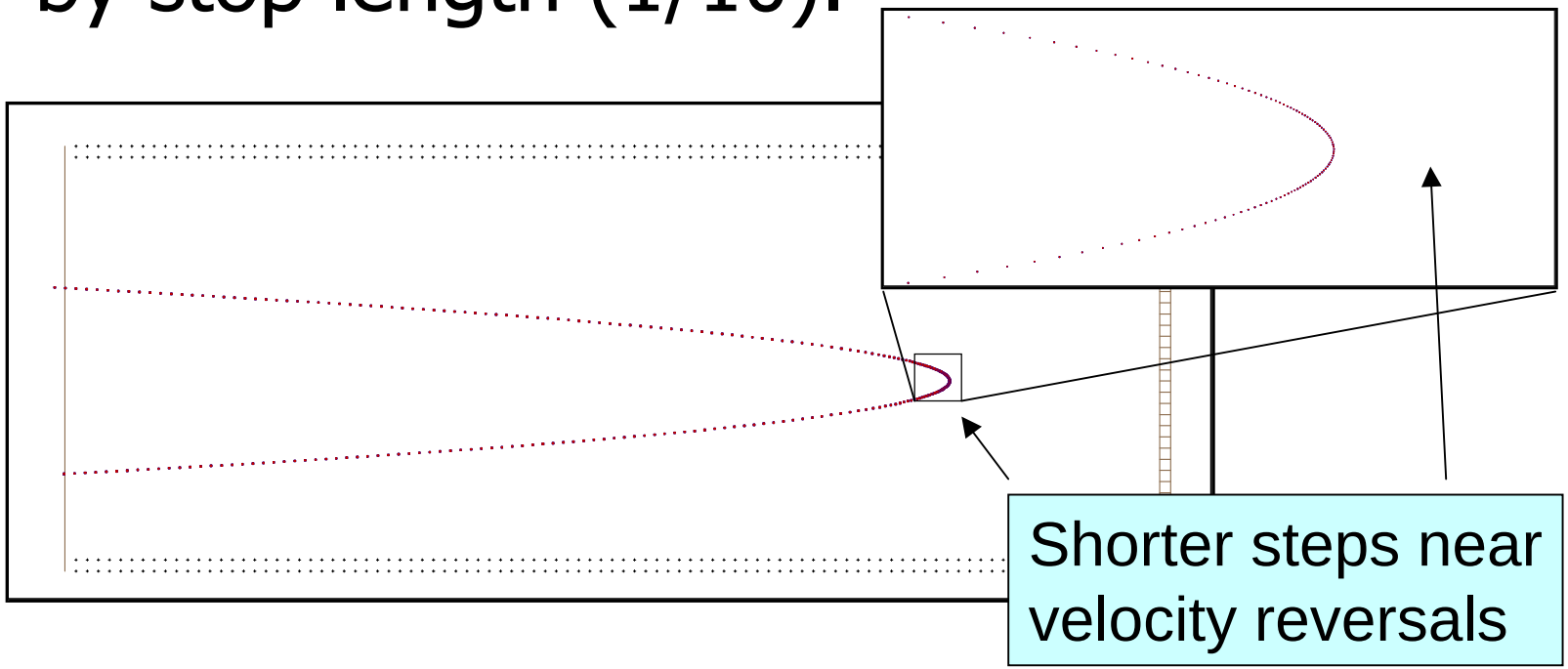
Numerical Integration

- SIMION uses a highly modified 4th order Runge-Kutta method orientated to fixed distance step integration.



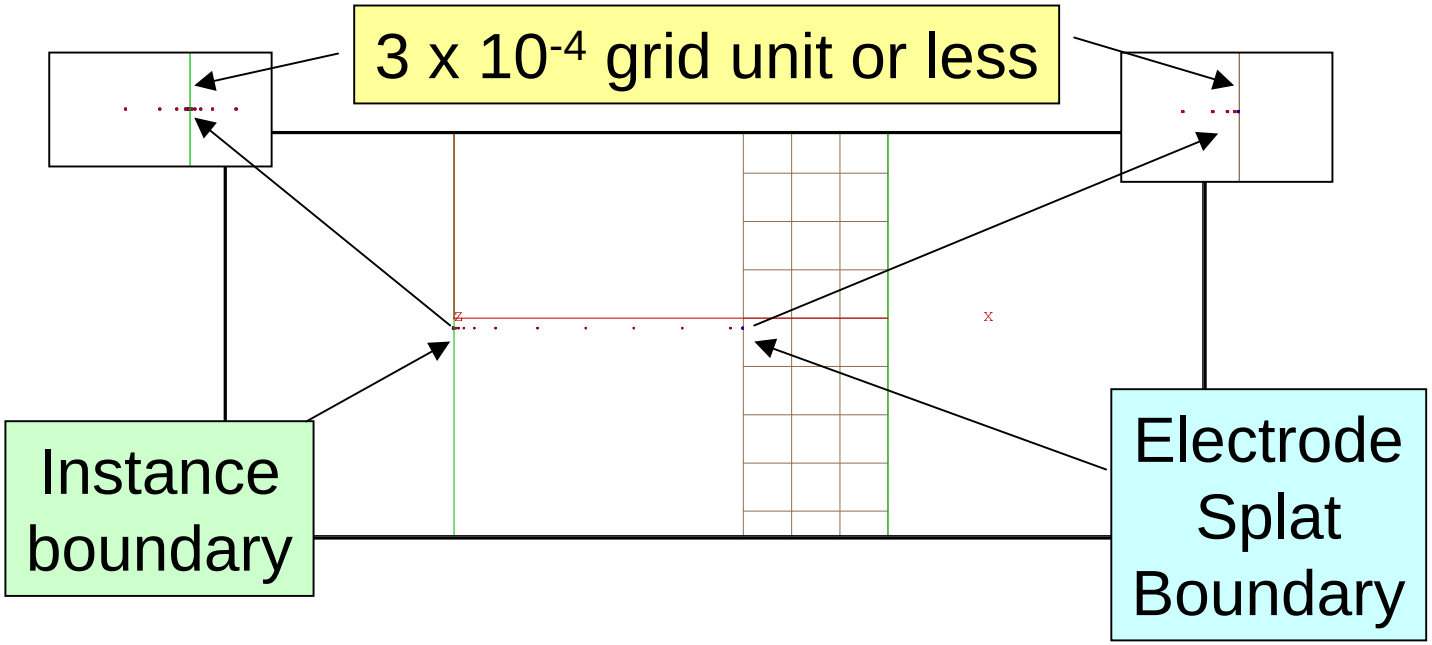
Numerical Integration

- Fixed distance step integration is modified by stop length (1/10).



Binary Boundary Approach

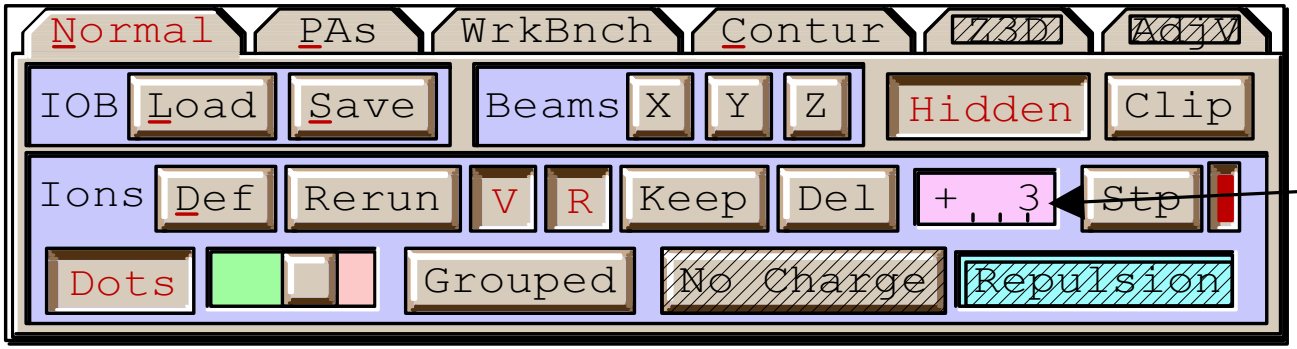
- Detect, leap back, and halve the time step is used to approach boundaries.



Binary Boundary Approach

- Detected boundaries:
  - Instance boundaries
  - Electrode (splat) boundaries
  - Velocity reversals
  - Regions of higher coefficient of variation of acceleration -- field discontinuities (grids) or time varying fields (step changes in potentials).

Adjusting Trajectory Quality



Trajectory Quality Panel

Trajectory Quality	Distance Step in gu	Minimum Step in gu	Stop Length	Binary Boundary	CV Upper Limit
-n	1/(1+n)	NA	yes	no	NA
0	1	NA	yes	no	NA
3 (default)	1	$1/(3 \times 10^4)$	yes	yes	1/3
$1 \le n \le 100$	1	$1/(n \times 10^4)$	yes	yes	1/n
$100 < n$	1/(1+(n-100))	$1/(n \times 10^4)$	yes	yes	1/n

Trajectory Quality

- Positive values of trajectory quality generally give the most accurate trajectories.
  - The default value of 3 represents a good starting compromise.
  - Higher values can improve accuracy at the cost of speed.
  - Vary positive quality to evaluate accuracy.

Trajectory Quality

- Zero or negative values of trajectory quality give the fastest computations.
  - The value of 0 provides the fastest and least accurate trajectories.
  - Increasingly negative values improve accuracy to a point.
  - Negative values are useful for flying ions in groups or when history is lost (damping).

Trajectory Quality hints

- Flying ions singly (most efficient)
  - Use default value of 3
  - Test for consistency with higher values
  - 0 or negative values have no boundary detect
- Flying ions in groups (can be very slow)
  - Use 0 or negative values for speed
  - Positive values can be VERY slow (most constrained ion slows all others down)