

4.3.1 - RNA Hydrolysis

Parameters

| Parameter Name | Variable | Default Value | Parameter Range | Description |
|----------------|-----------------------------|------------------|-----------------------------|---|
| FRAG_UR_D0 | Unknown macro: 'mathinline' | 1 | >0 | minimum length of fragment |
| FRAG_UR_DE_LTA | Unknown macro: 'mathinline' | NaN ¹ | Unknown macro: 'mathinline' | geometry of the fragment: 2=surface-diameter, 3=volume explicitly specified (NaN), depends logarithmically on |
| FRAG_UR_ETA | Unknown macro: 'mathinline' | NaN ¹ | Unknown macro: 'mathinline' | intensity of fragmentation, breaks per unit length; if non-zero, is determined by the correlation coefficient and an expectation value and an expectation fragment size, if size selection is enabled |

¹ NaN stands for "Not a Number" and marks the uninitialized state of a parameter

Algorithm

Frequencies of fragment sizes produced by a uniform random fragmentation process have demonstrated to fall along Weibull distributions, if the fragmentation thermodynamics depends on the molecule size:

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Scale parameter represents the intensity of fragmentation (i.e., breaks per unit length), and—as a determinant of the mean expected fragment size—is assumed to be constant across molecules of different lengths for fragmentation protocols where the number of produced fragments depends on the molecule length. Shape parameter reflects the geometric relation in which random fragmentation is breaking a molecule (e.g., fragmentation on the linear chain of nucleotides, the volume, etc.).

Unknown macro: 'mathinline' corresponds to uniform fragmentation, which splits uniformly the surface, and

The Flux Simulator uses a 3-step algorithm to tokenize a molecule; first, geometry

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and the number

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of fragments that are obtained from the molecule are determined. We found empirically that parameter

d depends logarithmically on

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, the length of the molecule that is fragmented

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. The number of fragments produced from a specific RNA molecule is determined by

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, where Unknown macro: 'mathinblock' is the expectancy of the most abundant

fragment size, computed from h and the gamma-function

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of

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:

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Second,

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breakpoints are sampled uniformly from the interval [0;1], resulting in relative length fractions

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for all

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fragments. Third, relative fragment sizes

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are transformed from unit space to sizes

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that follow

a Weibull distribution of shape

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by:

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where

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is a constant of the transformation to ensure that the sizes of the

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fragments sum up exactly to the given molecule length

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. Latter transformation produces a slightly distorted Weibull distribution for the sizes

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, however the deviation is sufficiently small to be neglected in our applications.