Cost-effective sampling in large scale scientific simulations is challenging because of the high dimensional parameter space, discontinuous simulation outcomes and expensive computation for each simulation.

**Discontinuities-aware sampling**

If discontinuities are known, more samples should be put in the discontinuous area.

**Discontinuity analysis**

Program outputs correlate with frequencies of executed paths.

**Example:**

Brusselator model of autocatalysts reactions:

\[ R_1: x \rightarrow y \]
\[ R_2: 2y + z \rightarrow 3z \]
\[ R_3: y \rightarrow z \]
\[ R_4: y \rightarrow z \]

4 reactions are coded in the program with 2 branches, 4 paths.

**Idea:** By reverse engineering the conditions of important divergent paths for different sample executions, we can locate the discontinuities in input space.

**Reference:**