

# Algorithms

# Exact Algorithm

## Origins of Derivation and Brief Discussion

- Time ordered product expansion (TOPE) can be used to derive a simulation algorithm<sup>1</sup>.
- A key defining characteristic is the time warping equation.
  - Exponential distribution for waiting times.
- The exact algorithm becomes slow for large system.
- Rule firings (rewrites) must be in order.
- Good for small systems and easy to implement.

### Exact Hybrid Parametrized SSA/ODE Algorithm

```
factor  $\rho_r([x_p], [y_q]) = \rho_r([x_p]) * P([y_q] | [x_p]);$   
while  $t \leq t_{max}$  do  
  initialize SSA propensities as  $\rho_r([x_p]);$   
  initialize  $\rho^{(total)} := \sum_r \rho_r([x_p]);$   
  initialize  $\tau := 0;$   
  draw effective waiting time  $\tau_{max}$  from  $\exp(-\tau_{max});$   
  while  $\tau < \tau_{max}$  do  
    solve ODE system, plus an extra ODE updating  $\tau;$   
     $\frac{d\tau}{dt} = \rho^{(total)}(t);$   
  draw reaction  $r$  from distribution  $\rho_r([x_p]) / \rho^{(total)};$   
  draw  $[y_q]$  from  $P([y_q] | [x_p])$  and execute reaction  $r;$ 
```

Algorithm 1

1. (Mjolsness, 2013)