Improving the Exact Algorithm

Proposal for potential points of parallelization

- Parallelizable over propensity calculations.
- Parallelizable over propensity sums.
- Parallelizable over ODE solving when appropriate scaling and resources are available.
- Reactions must be still fired in order.
- Has potential for quick testing of medium-sized systems.
- Could be used to incorporate hierarchical parallelism in the approximate algorithms.

Parallel Exact Hybrid Parametrized SSA/ODE Algorithm

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

Deriving the Approximate Algorithm

Operator splitting and approximation.

- A method to approximate e^{tW} is a first-order operator splitting algorithm that imposes a domain decomposition by means of an expanded cell complex.

- The decomposition corresponds to summing operators, $W = \sum_{(d)} W_{(d)} = \sum_{(d,c)} W_{(c,d)}$ over pre-expansion dimensions *d*, and cells *c* of each dimension where $d \downarrow$ means we multiply from right to left in order of highest dimension to lowest:

$$e^{tW} \approx \left(\prod_{d\downarrow} e^{\frac{t}{n} W_{(d)}} \right)^{n \to \infty}$$

$$e^{t'W_{(d)}} = \prod_{c \subset d} e^{t'W_{(c,d)}} \quad \text{where} \quad [W_{(c,d)}, W_{(c',d)}] \approx 0 \quad \text{and} \quad t' \equiv \frac{t}{n}$$

$$W_{(c,d)} = \sum_r W_{r,c} \equiv \sum_r \sum_{\left\{ \substack{R \mid \varphi(R) = c, \\ R \text{ instantiates } r} \right\}} W_r(\, R \mid c, d)$$