Exact Algorithm

Origins of Derivation and Brief Discussion

- Time ordered product expansion (TOPE) can be used to derive a simulation algorithm¹.
- 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 \le 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

Cell Complex

The motivation for the expanded cell complex.

- A cell complex¹ C is a collection of mathematical n-dimensional n-cells, and all lower-dimensional cells that make up their boundaries.
- For any k-cell, ∂ is the operator that returns the cell's boundary if it exists.
- A cell complex can also be represented as a graph.

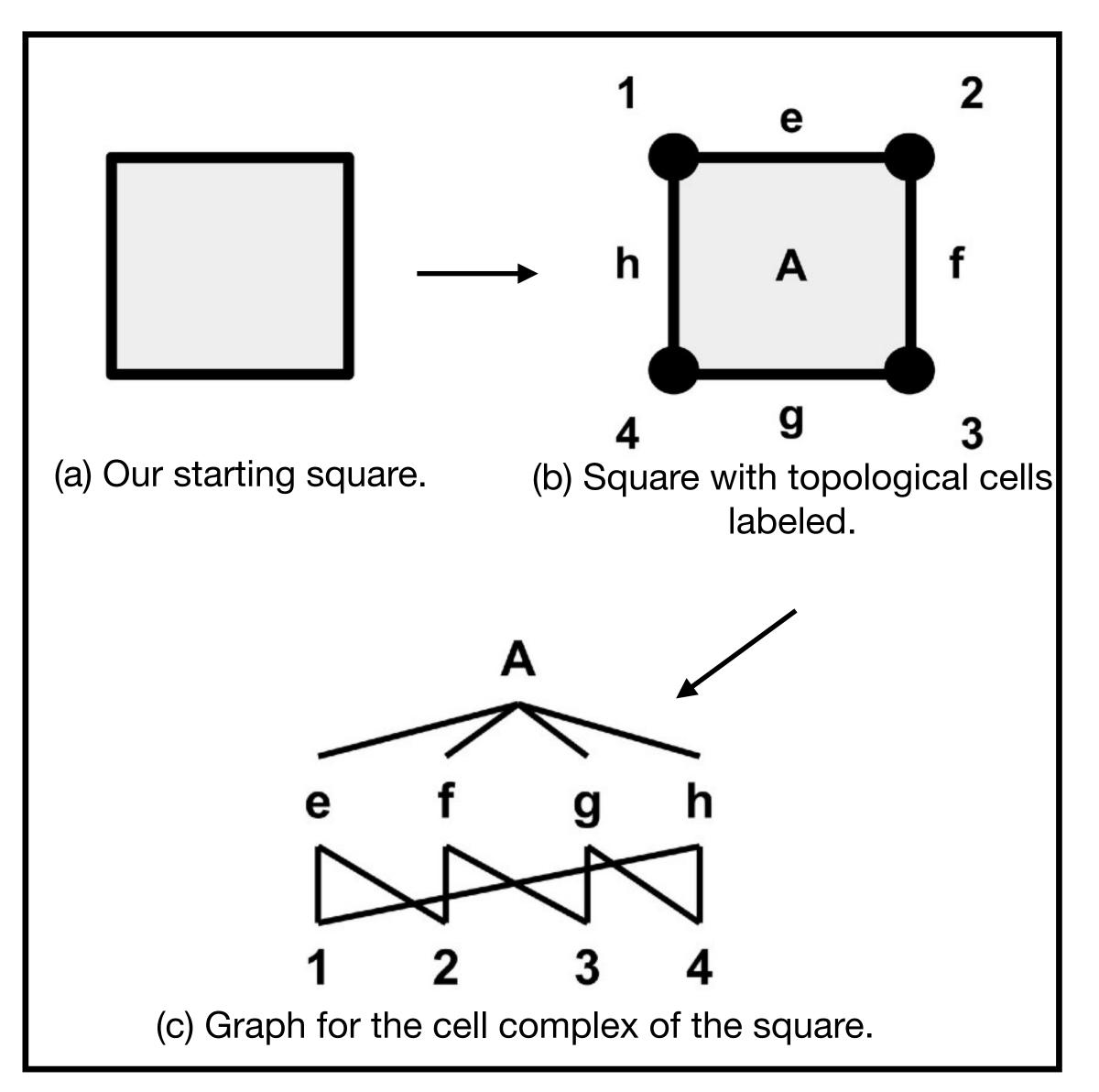


Figure 5