The Reaction Grid

Context for the cell list

- A cell list[1] is a data structure to find combinations of objects within a given cut-off distance of each other.
    - Cell size defined using a user defined reaction radius.
    - Enables efficient geometric search of nearby objects and combinatorial matching of nearby components.
- The cell list is integral in the incremental update.
- The cell list can be used in the rule mapping function φ.
- Other potential methods are bounding volume hierarchies[2], k-d trees[3], etc.

1. (Slattery, 2022); 2. (Ericson, 2004); 3. (Bentley, 1975)

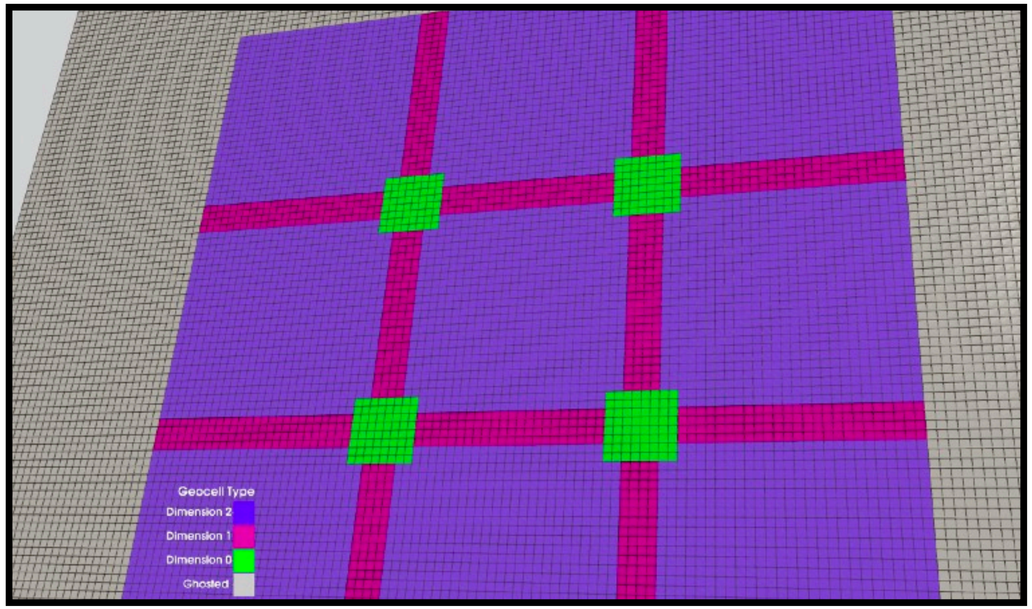

Figure 17: ECC overlaid with a “reaction grid” from a cell list and “ghost cells”.

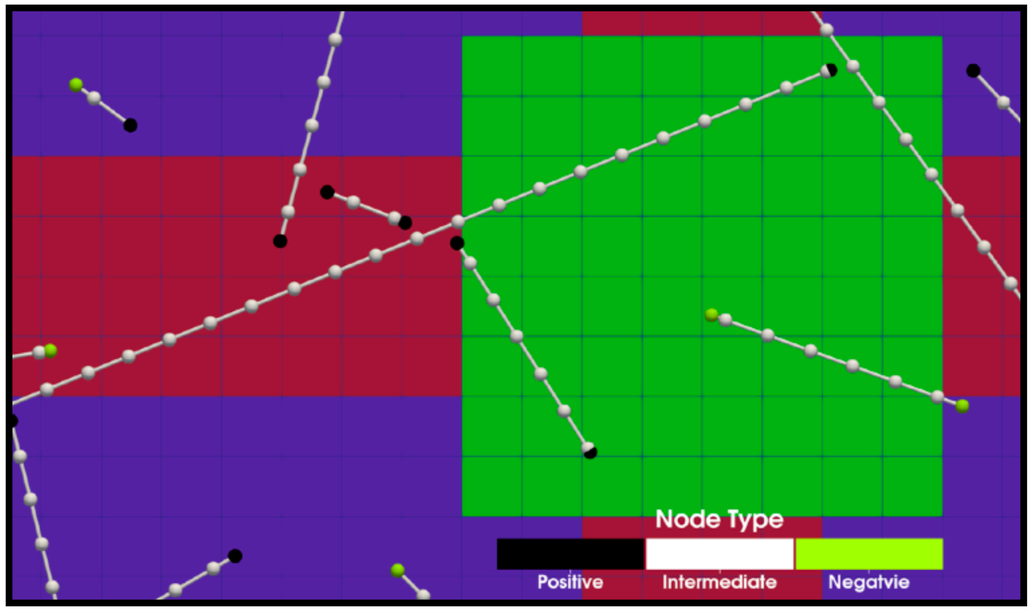

Figure 18: Zoomed in version with graph rules shown.

Original Approximate Algorithm

The first attempt at the approximation

- Differing dimensions can be processed separately.
- Potential for parallel processing over dimension and within a geometric cell.
- Reactions (rules) are spatially local and may be fired out of order at the cost of accuracy.

Original Approximate Spatially Embedded Hybrid Parameterized SSA/ODE Algorithm

while $t \leq t_{max}$ **do**
  foreach *dimension* $d \in \{D_{max}, D_{max} - 1, \ldots, 0\}$ **do**
    using function φ *map rule instances to the geocells of the expanded cell complex*;
    ParFor expanded geocell $c_i \in ExpandedCellComplex(d)$ **do**
      run Exact Hybrid Parameterized SSA/ODE algorithm for Δt in c_i;
  $t \mathrel{+}= \Delta t$;

Algorithm 2

- Good for larger simulations.
- Requires more details to fully address the problem.

(Medwedeff and Mjolsness, 2023)