Subgraph Pattern Recognition

Finding Graphs of the LHS.

- To find subgraph matches isomorphic to our search pattern, we find injective graph homomorphisms.
- For the search pattern, a rooted spanning tree (RST) is generated.
- The RST and other constraints are used to find matches in the graph.
- Combinations of search patterns are used to find matches for LHS graphs.

Sources: (Valiente, 2021), (Carletti et al., 2018), Medwedeff and Mjolsness) and more in thesis.

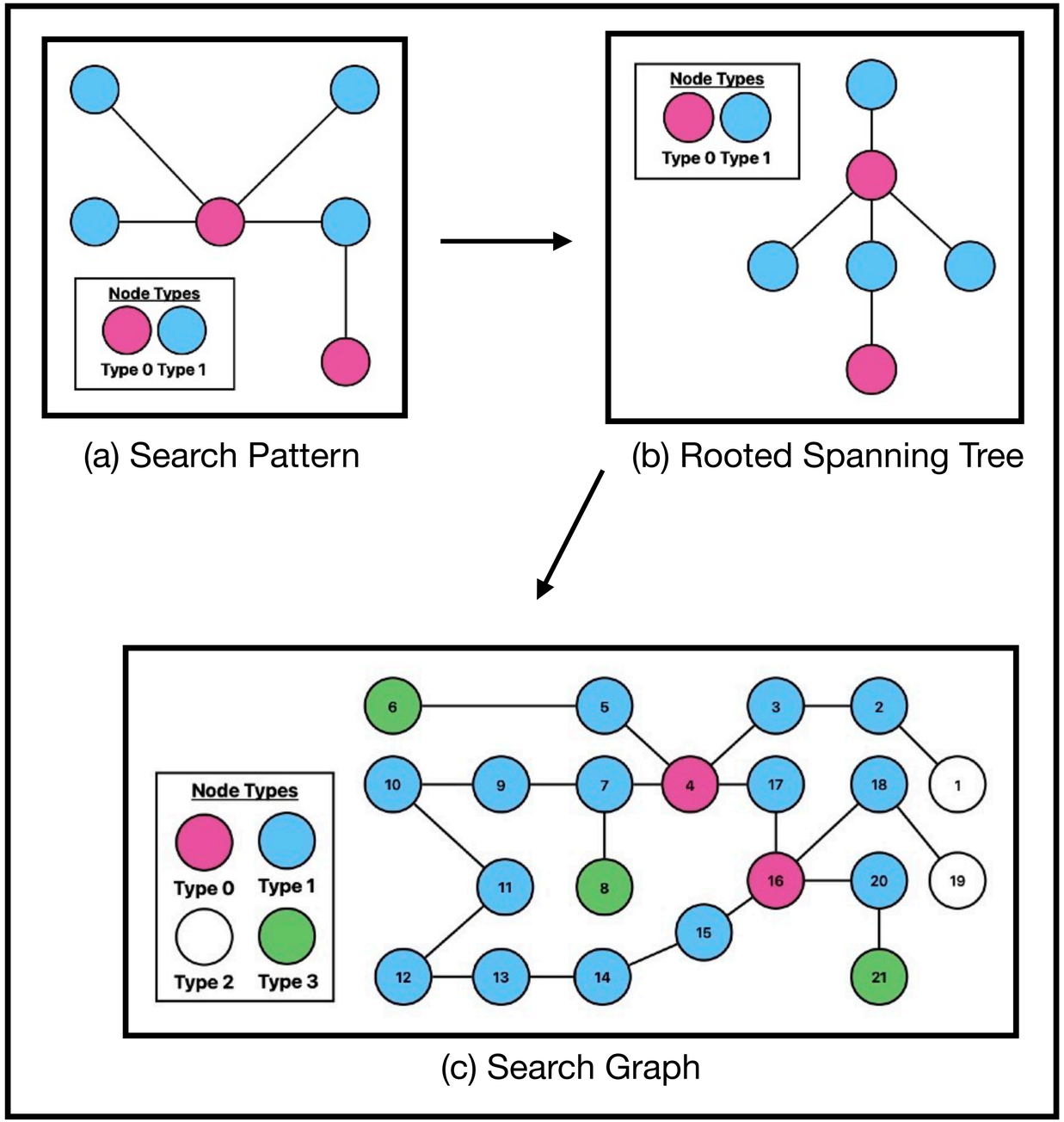

Figure 23: Search Process

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)

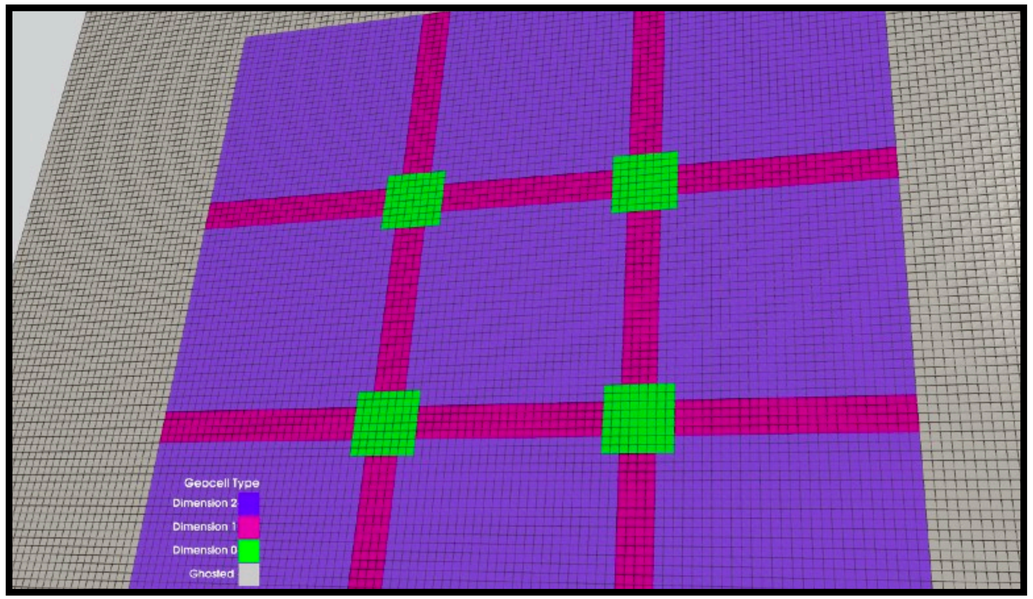

Figure 24: ECC overlaid with a “reaction grid” from a cell list and “ghost cells”.

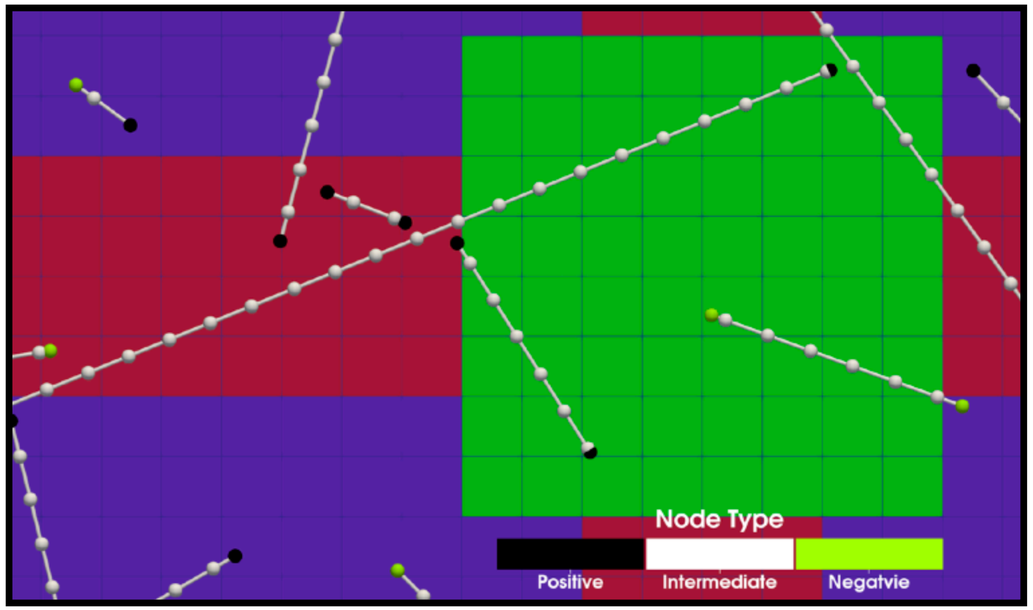

Figure 25: Zoomed in version with graph rules shown.