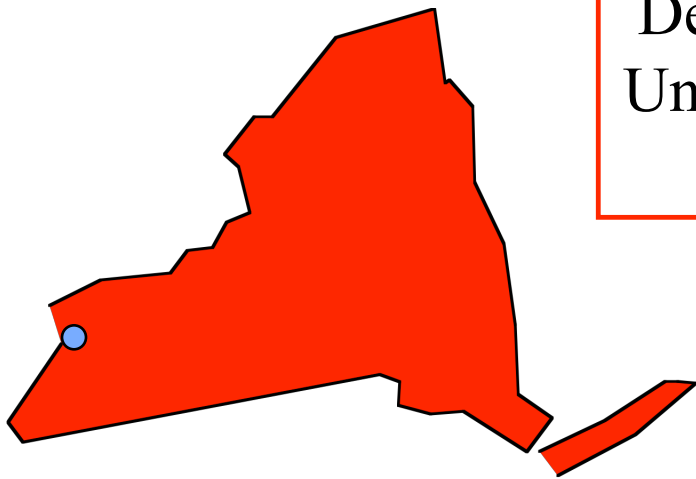


All About Potentials and Iterators

David A. Kofke

Department of Chemical Engineering
University at Buffalo, State University
of New York



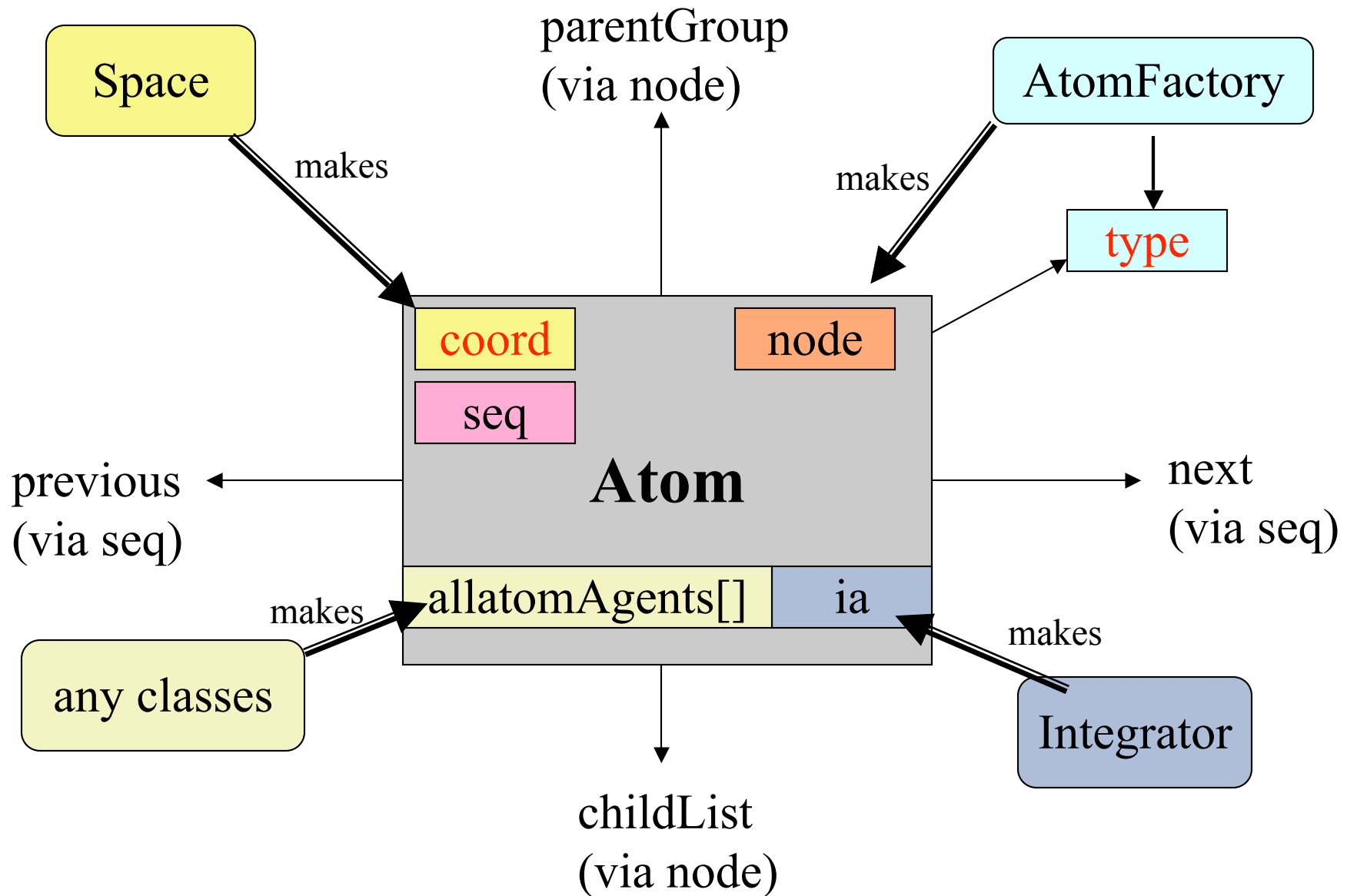
Potential

- Top-level simulation element
 - Species, Potential, Integrator, Controller, Meter, Device, Display
- Defines methods and holds fields that define interactions between atoms
- Potential is responsible for knowing the atoms to which it applies
 - Uses appropriate iterators for this purpose
- Hierarchical structure that parallels structure of species hierarchy

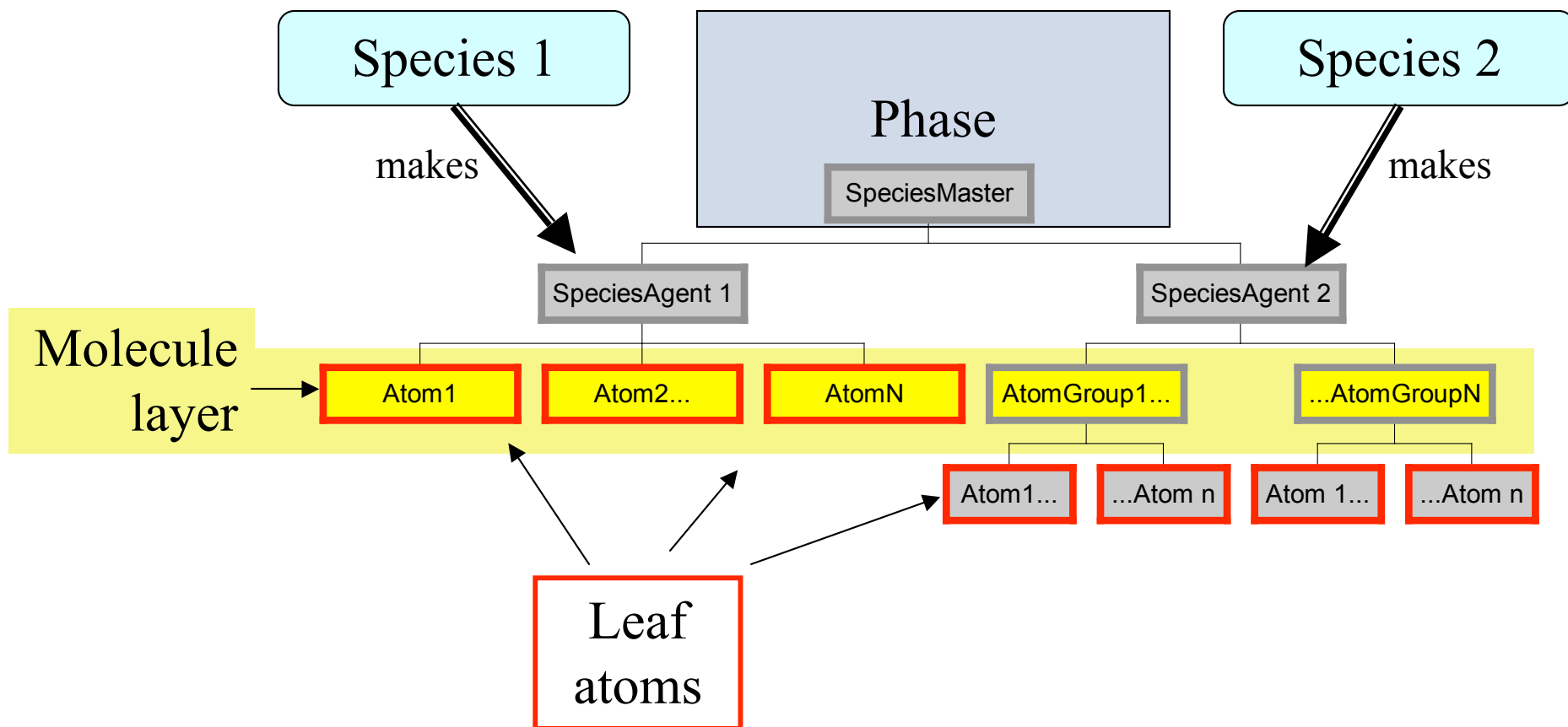
Atom

- Corresponds to a physical atom (in simplest case)
- Holds data relating to
 - Spatial coordinate (position and/or momentum)
 - Atom type
 - Position in atom hierarchy
 - Position in atom sequence
- Can also hold auxiliary data
 - Agents from other classes
 - Parameters specified by other classes (in type field)
 - Lists of other atoms for use by other classes

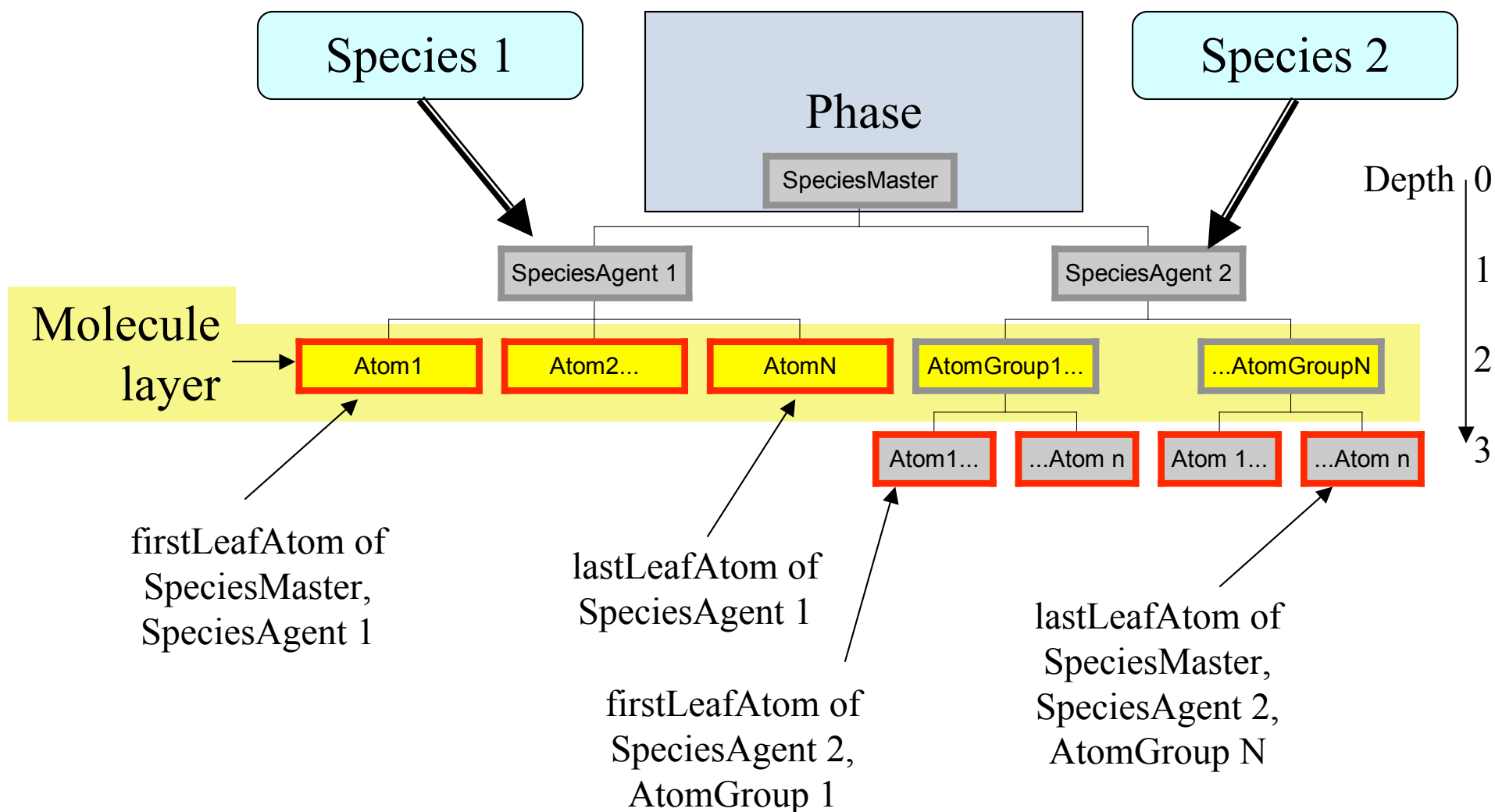
Atom Fields



Species Hierarchy

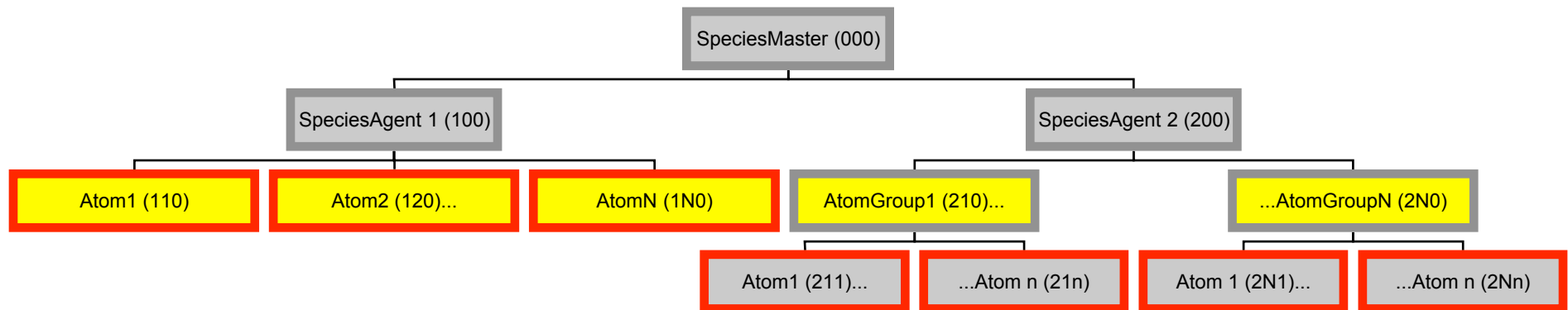


Species Hierarchy



Ordering

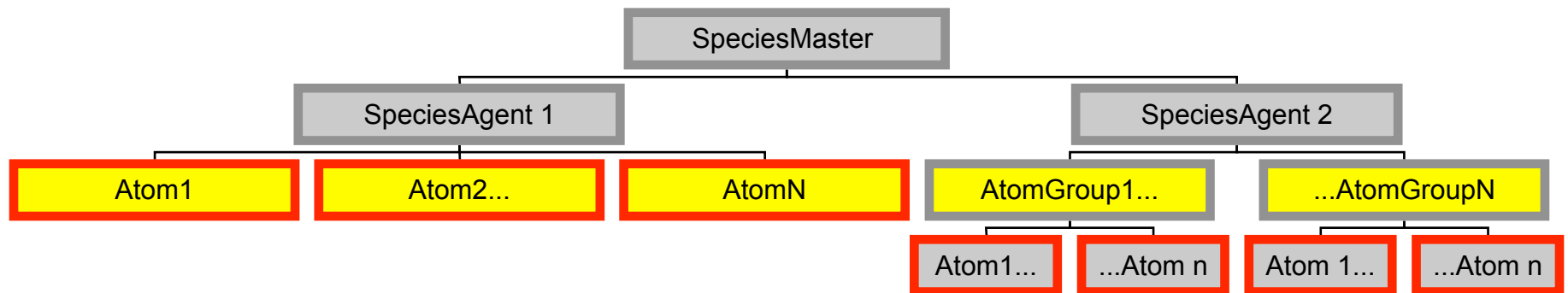
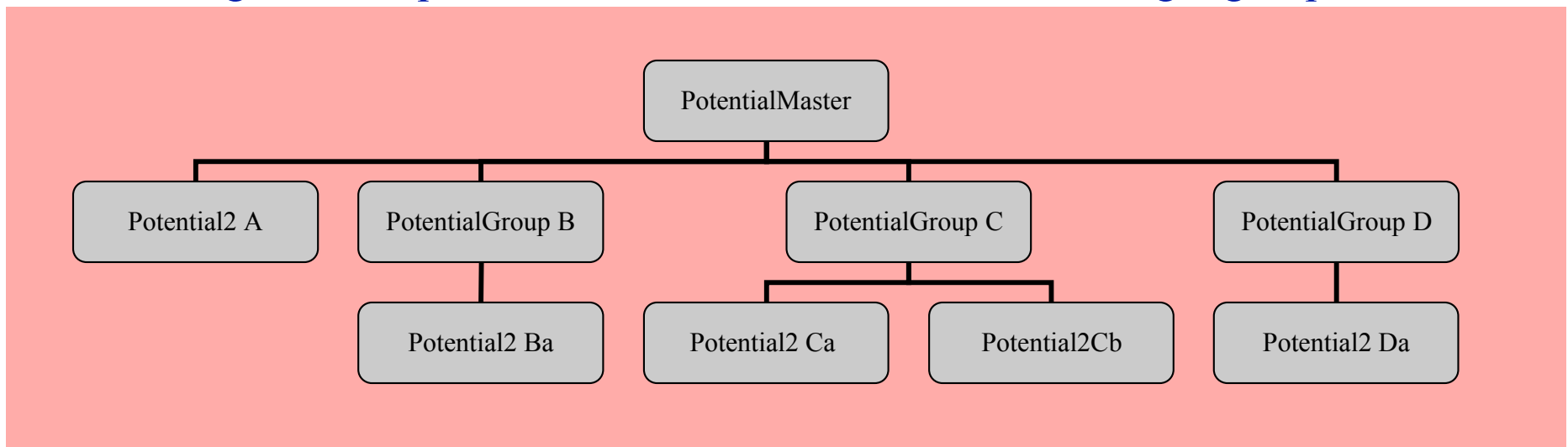
- Atoms are ordered to facilitate looping through them



- $000 \rightarrow 100 \rightarrow 110 \rightarrow 120 \rightarrow \dots \rightarrow 1N0 \rightarrow 200 \rightarrow 210 \rightarrow 211 \rightarrow \dots \rightarrow 21n \rightarrow \dots \rightarrow 2N0 \rightarrow 2N1 \rightarrow 2Nn$
- Looping might be required to go up or down list, from any point, and at any level in hierarchy
- Ordering might be fixed, or might depend on spatial configuration (cell neighbor list)

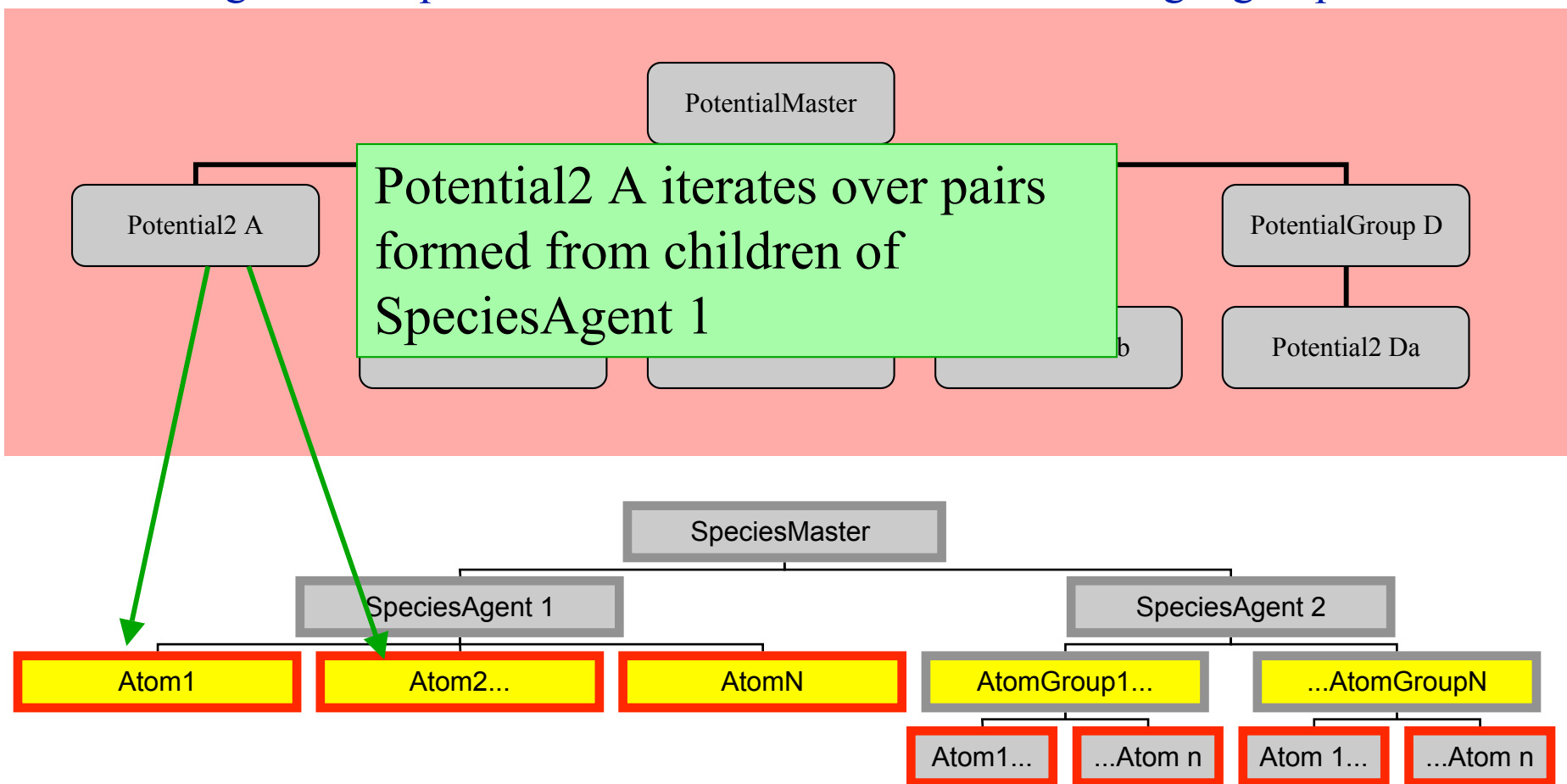
Potential Hierarchy

- Potential hierarchy parallels species hierarchy
 - Higher-level potentials define interactions between larger groups of atoms



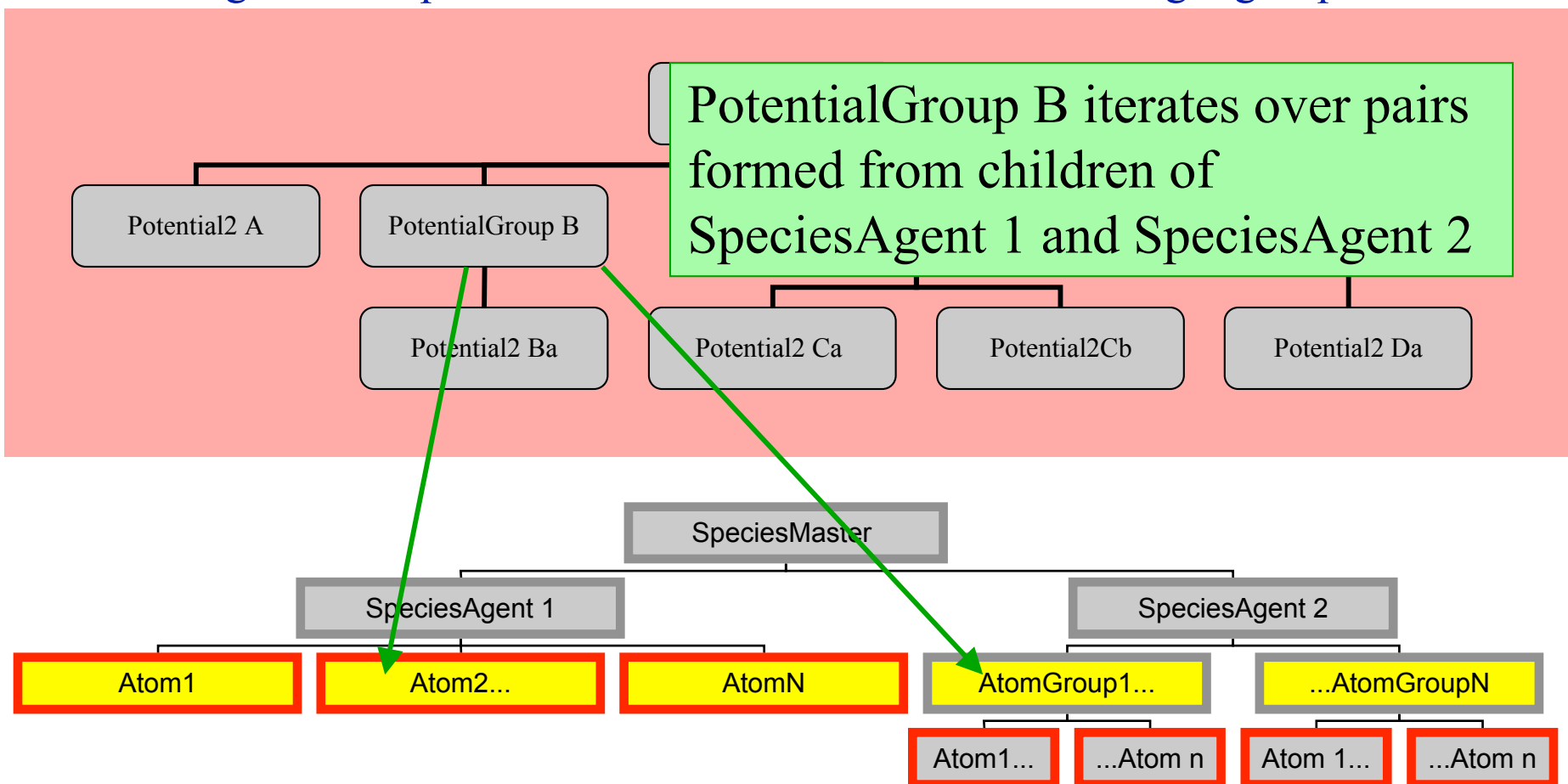
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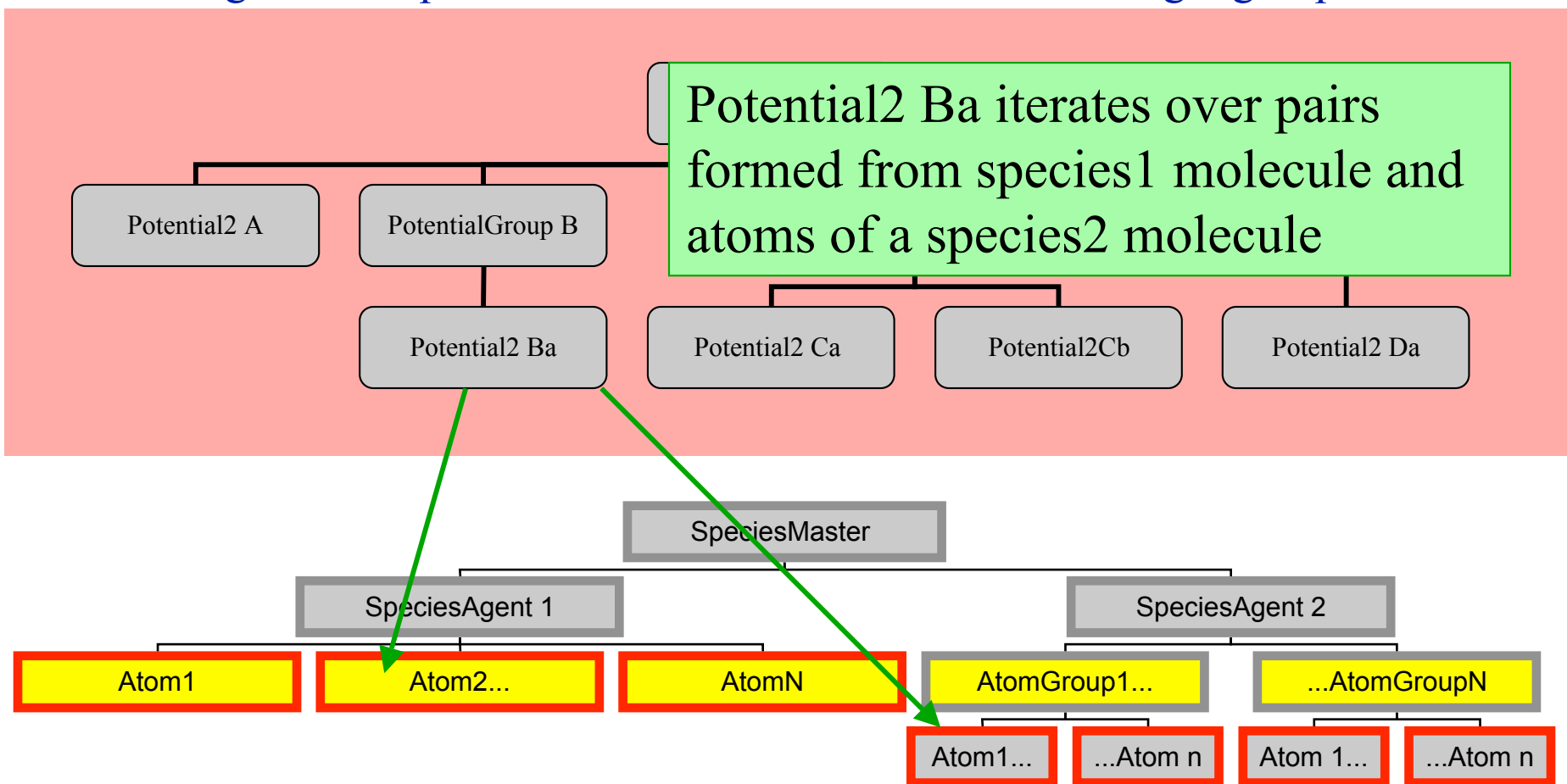
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Potential Hierarchy

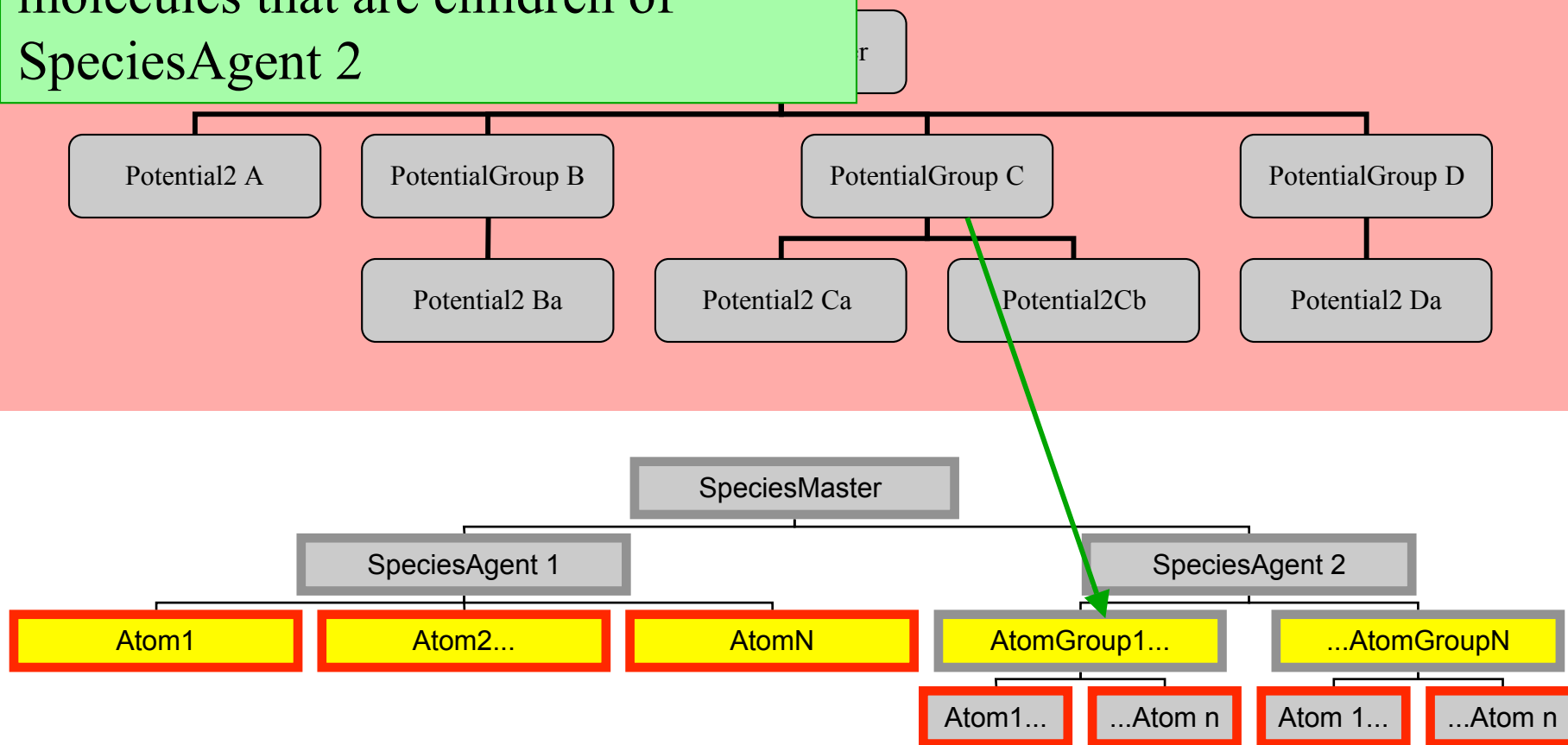
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Potential Hierarchy

- Potential hierarchy parallels species hierarchy

PotentialGroup C iterates over single molecules that are children of SpeciesAgent 2

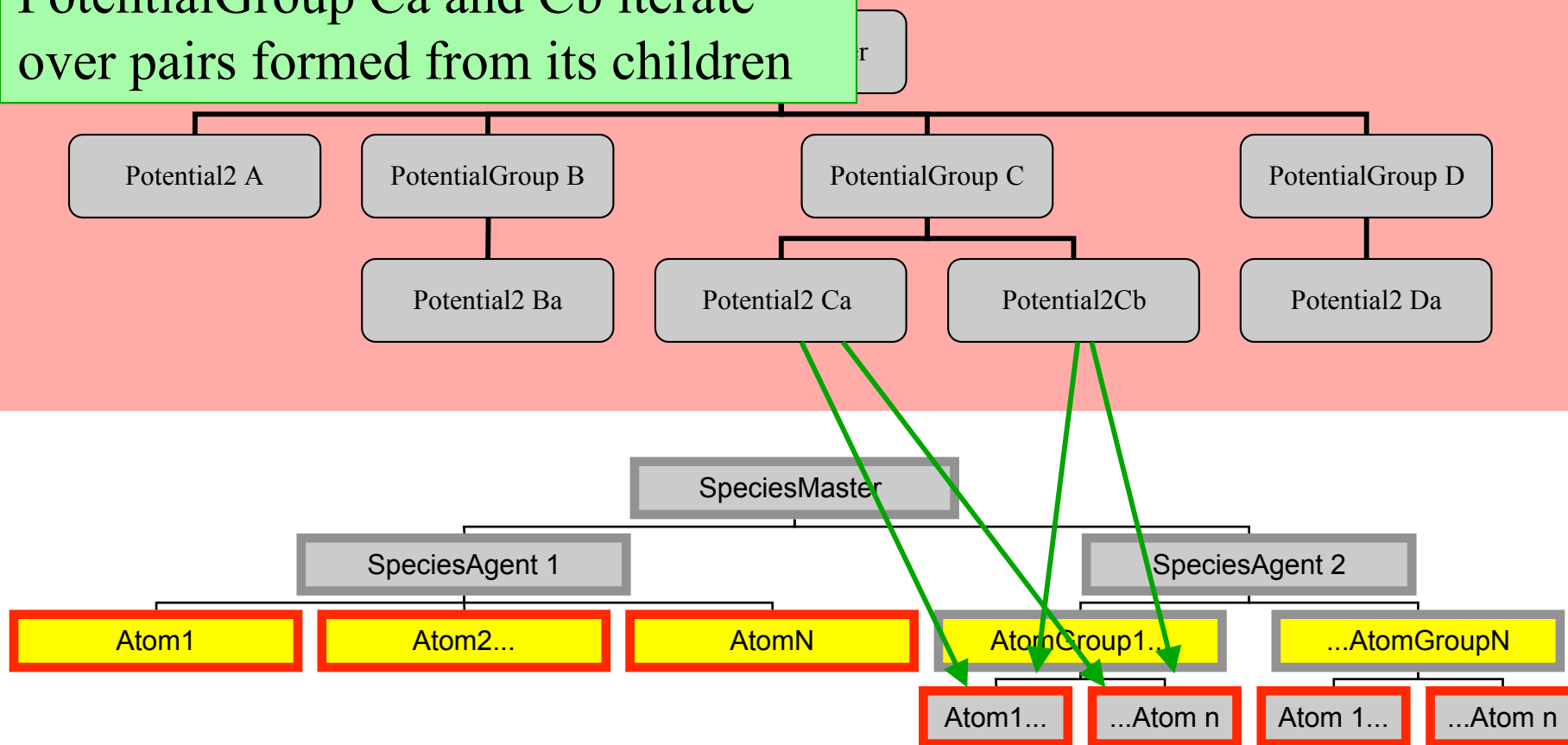


Potential Hierarchy

- Potential hierarchy parallels species hierarchy

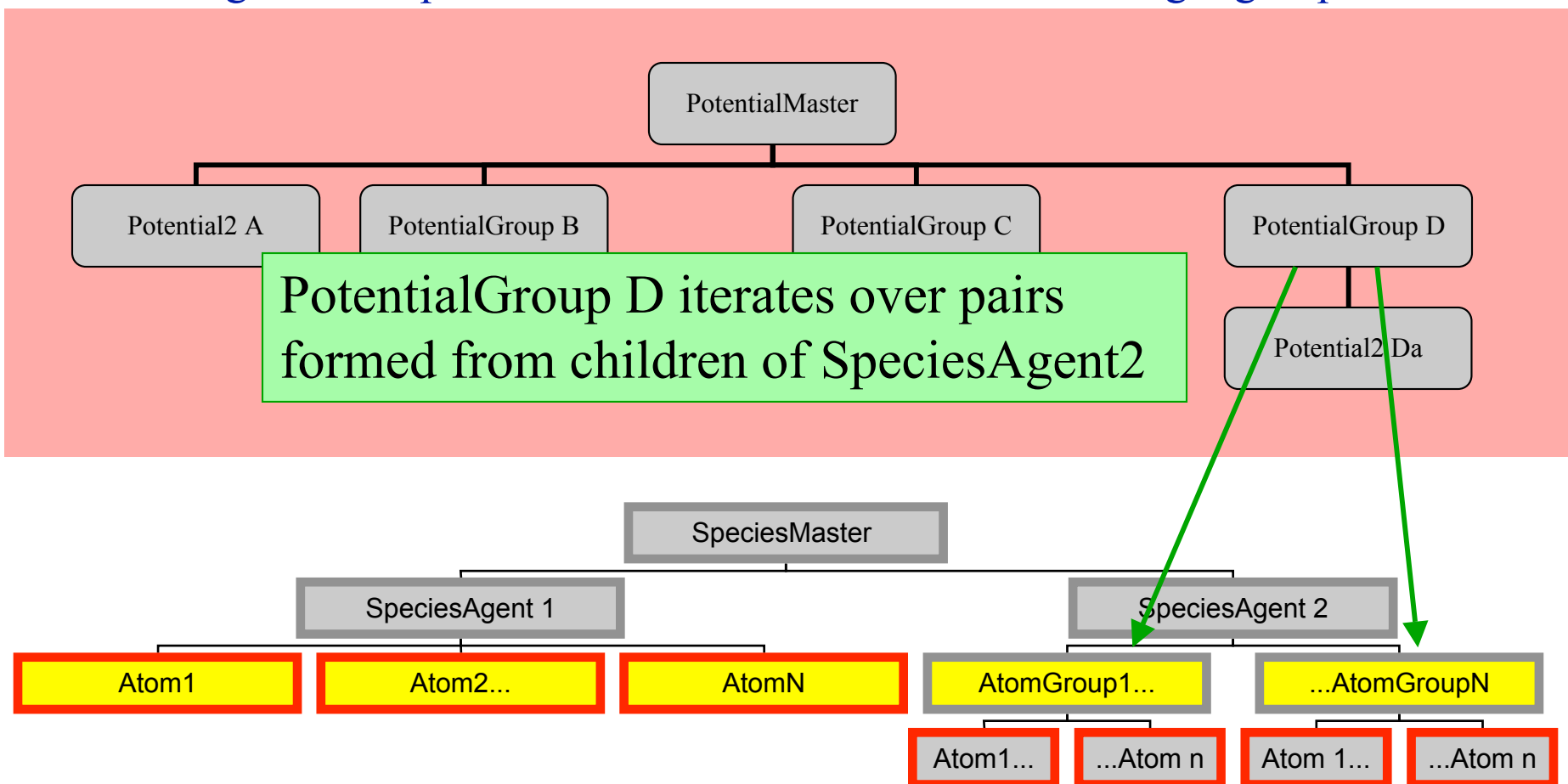
For a given species-2 molecule, PotentialGroup Ca and Cb iterate over pairs formed from its children

Iterations between larger groups of atoms



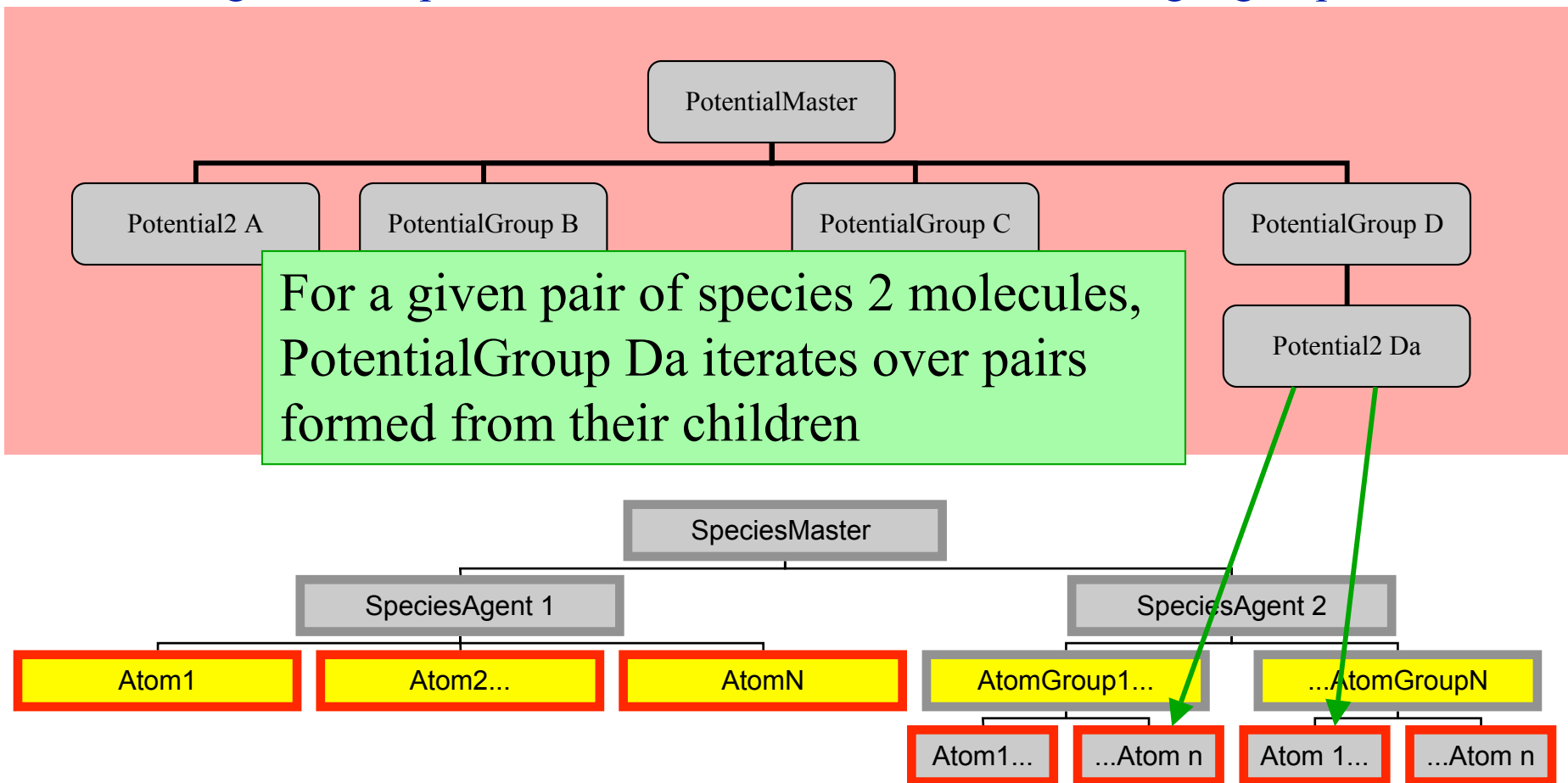
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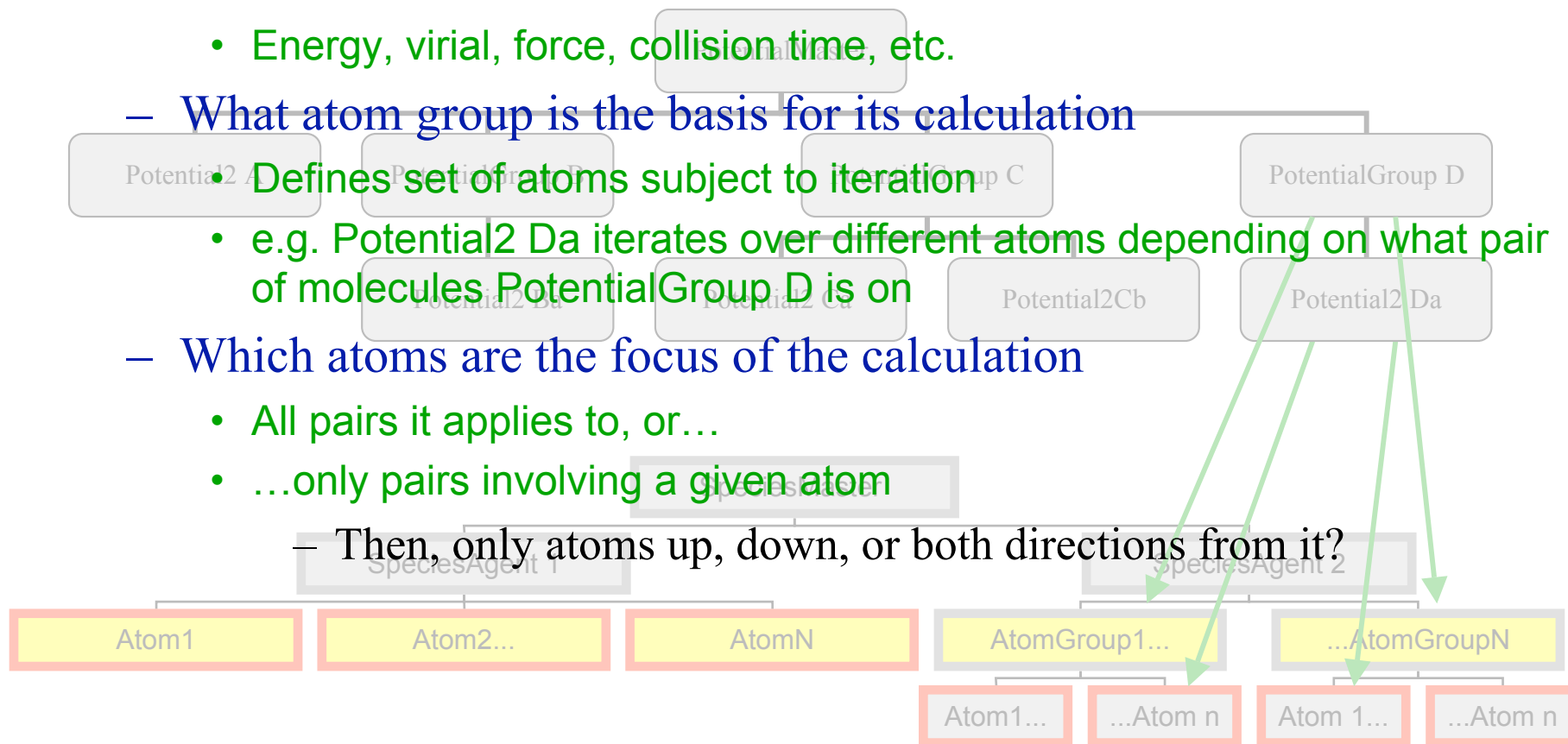
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Using the Potentials

- To get information from potential, we need to tell it
 - What calculation is to be done
 - Energy, virial, force, collision time, etc.
 - What atom group is the basis for its calculation
 - Defines set of atoms subject to iteration
 - e.g. Potential2 Da iterates over different atoms depending on what pair of molecules PotentialGroup D is on
 - Which atoms are the focus of the calculation
 - All pairs it applies to, or...
 - ...only pairs involving a given atom



– Then, only atoms up, down, or both directions from it?

Using the Potentials

- Basic format (current)

Current form

```
potential.set(basis).calculate(iteratorDirective,  
                               energyCalculation);
```

New form

```
potential.calculate(basis, iteratorDirective,  
                   energyCalculation);
```

- Arguments
 - **basis**: Defines set of atoms subject to iteration
 - **iteratorDirective**: specifies type of iteration desired
 - **energyCalculation**: contains method to perform desired calculation
- Process (examine code, but currently under revision)
 - calculate method sets up potential's iterator for looping, and instructions in energyCalculation are performed

Iterator Directive

- IteratorDirective holds fields that direct iteration
 - Key attributes (among a few others)
 - direction
 - UP, DOWN, BOTH, NEITHER
 - atom
 - iteration performed in reference to atom, if not null
- Basis defines the source of atoms for the iterator
 - Within a given basis, iterator may loop over atoms in different ways
 - Depends on iteratorDirective
 - Depends on design of iterator
 - All children
 - Children two (e.g.) steps deeper
 - “neighbors” only
 - Only ones bonded/not bonded to an atom
 - Only first or last child
 - Etc.

Using an Iterator

- Perform actions on iterates (pass atoms to action)

```
iterator.reset();  
while(iterator.hasNext()) {  
    Atom atom = iterator.next();  
    //do something with atom  
}
```

- Pass action to iterator

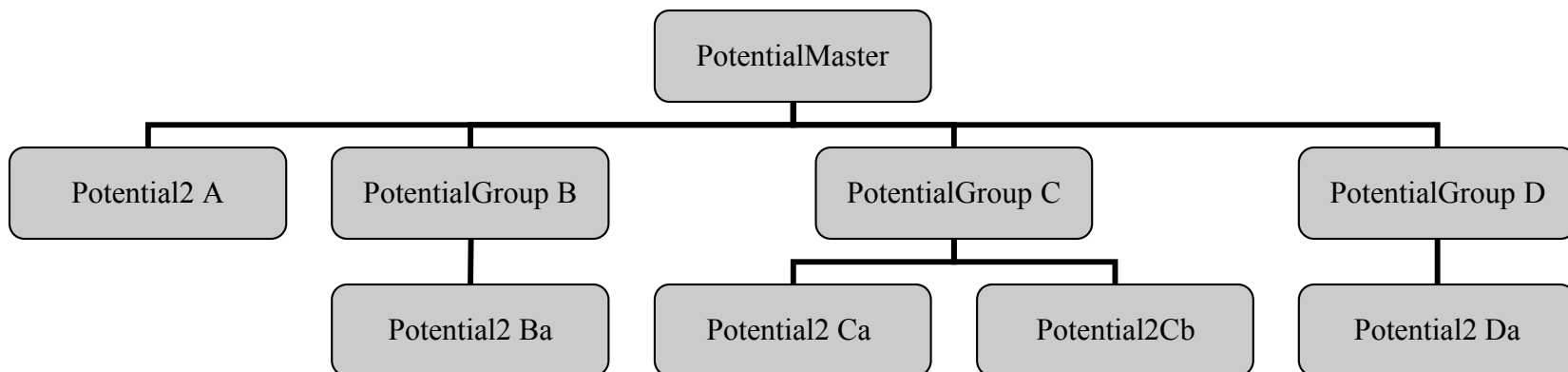
```
AtomAction action = ...//define action  
iterator.all(basis, directive, action);  
    //performs action on directed atoms  
    //in basis
```

Threading in Java

- Independent process of calculation
 - In single-processor platforms, control moves from one thread to another in unpredictable ways
 - In multi-processor platforms, each processor can be running a different thread
- Different threads may be using the same data, or the same instances of objects
 - Must be careful that threads do not interfere or corrupt each other's activities
- Possible paradigm for conducting parallelized simulations
 - Different parallel-tempering phases running on individual threads
 - Simulations on a single phase might use different threads to advance simulation in different regions of space

Problem with Multithreading

- Only one potential hierarchy is instantiated
- Threads running in different phases operate on hierarchy simultaneously
 - E.g. Thread 1 has Potential2 A iterating over atoms in its phase
 - In the middle of this, Thread 2 comes in and resets iteration for atoms in another phase



Solutions to Multithreading Problem

- Construct identical potential hierarchies, each devoted to a single thread
 - Complicated by need to ensure that potentials always remain identically defined across all instances
 - Modifications (change in parameters or addition/removal of a potential) must be transmitted to all instances
 - Difficulty can be alleviated by defining hierarchy of potential agents
 - Agents have individual iterators
 - Agents refer to single, common hierarchy of potentials for their definition
- Use stateless iteration (demonstration)
 - Pass calculation to iterator
 - Much easier, less error-prone to program, understand, and maintain
 - Performance issues?
 - Current modifications are now following this path