CS 594 - Final Presentation: Chemical Computation

Ty Vaughan

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THE UNIVERSITY OF TENNESSEE
KNOXVILLE

Chemical Computation: Overview

1. **Brief History**
2. What is Chemical Computation?
3. Real vs Artificial Chemical Computation
4. Programming Paradigm of Chemical Computation
5. Artificial Chemical Computation Example
6. Current Technology
7. Future Advances
8. Conclusion

Brief History

In the early 1900s, scientists were still gaining an understanding of how to quantify certain chemical properties and interactions

In the 1920s, theoretical calculations for chemical and quantum physics were being published that accelerated progress

- Schrodinger's wave equation
- Hiesenberg's establishment of quantum mechanics

As improvements in computer technology escalated by the 60s, research for how to program chemical experiments increased.

In 1971, Hendrickson published one of the first designs for a chemical program. The program was for computer-assisted synthesis of organic materials.

Brief History (Cont.)

More programs began to be developed, and in 1978, the two of the first companies dedicated to chemical computation hardware and software emerged.

From the 1980s on, many more companies and individuals began developing software tools for chemical computation.

Now, computational power is the main limiting force for many of the analyses able to be performed for chemical problems.

Unconventional computation with real chemicals grew as a field towards the end of the 1900s. One example is DNA computation, which was officially established with Adleman's 1994 publication of his DNA Hamiltonian path solver.

Advances in quantum computing are looked upon as one of the biggest improvements to further the field.

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What is Chemical Computation?

Chemical Computation is computation that focuses on modeling/computing chemical properties and reactions

It requires the programmer to define a basis of interpretation

- Can be straightforward
- Can be more abstract

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Two Types of Chemical Computation

There are two categories of chemical computation

1. Real Chemical Computation:
   - Use of actual molecules and chemicals in typical reactions
   - Use of a computer to simulate and compute chemical/quantum algorithms
2. Artificial Chemical Computation:
   - The application of the fundamental components of chemical reactions to abstractly perform problems.
   - The “Chemical Metaphor” for problem solving
   - Unconventional form of computation

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Chemical computation

How can we model chemical problems in software?

- Different aspects to consider
- Different elements to define
- Different approaches to be used
- Different models to apply

Aspects of Chemical Computation

Scope

1. Microscopic System:
   - A change of state in the overall system is described by a change of state of the individual components of the system.
   - Ex: Dittrich's prime number generator
2. Macroscopic System:
   - The state of the overall system is described by all components in the system
   - Ex: Dittrich's robot controller

Aspects of Chemical Computation

Determinism

1. Deterministic System:
   - Order of operations is known.
   - Ex: testing the properties of a chemical
2. Stochastic System:
   - Order of operations is not guaranteed
   - Ex: biological systems

Aspects of Chemical Computation

Openness

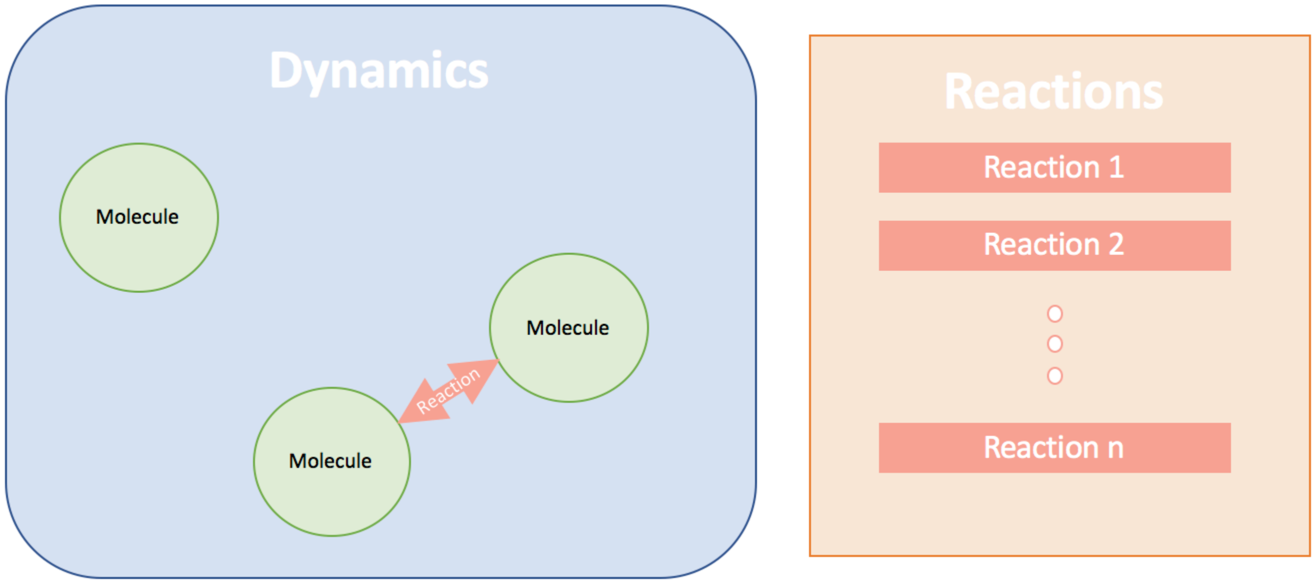
1. Open System:
   - Chemical reactions in the system do not need to be balanced.
   - Components can be introduced from or released back to the environment
2. Closed System:
   - Chemical reactions in the system are balanced
   - Components do not disappear from the system

Elements of Chemical Computation

There are three main elements that need to be defined:

1. Molecules:
   - these compose the state of the system and are the main components of computation in the system
2. Reactions:
   - these are the possible interactions that can occur between molecules and between molecules and the environment
3. Dynamics (Environment):
   - this determines how reactions begin, when they occur, and which reactions are possible

Elements of Chemical Computation



Approaches to Chemical Computation

There are two general approaches to setting up chemical computation problems:

1. Explicit definition of molecules and reactions
   - More favorable for simple systems where each reaction can be explicitly stated
2. Implicit definition of molecules and reactions
   - More favorable for complex, dynamic systems that can operate given only a few general rules
   - Larger reactions and molecules can be performed, composed of defined reactions and molecules

Models For Chemical Computation

The aforementioned aspects, elements, and approaches can be combined in five general models for chemical computation

1. Rewriting or Production Model
   - Sequences/patterns are used to represent the state of the system.
   - All reactions involve changing or rearranging the different sequences
   - Similar to how DNA computation is performed
     - Ex: Adleman's Algorithm for Hamiltonian paths
     - Ex: Lipton's SAT algorithm

Models For Chemical Computation

The aforementioned aspects, elements, and approaches can be combined in five general models for chemical computation

2. Arithmetic Model
   - Arithmetic symbols and operations represent molecules and reactions
   - Ex: Dittrich's Prime Number Generator
3. Abstract Automata Model
   - Molecules are represented by symbols and bits
   - Reactions performed are based on the molecule's symbols
   - Some molecules can represent the states of the automata, others can interact with the state molecules
   - Ex: Benenson's DNA FSM for enzymatic computation

Models For Chemical Computation

The aforementioned aspects, elements, and approaches can be combined in five general models for chemical computation

4. Assembler Automata Model
   - Assembler automata machine is used – highly parallel
   - Molecules, reactions, and environment are all specified and compete for CPU
   - Ex: Tierra – parisitic organism simulation
5. Lattice Model
   - Unit grid is generated, molecules exist within the grid
   - Molecules and reactions are specified, and the dynamics can be different for each lattice
   - Ex: Astor’s neural network development model

Advantages and Disadvantages For Chemical Computation

Advantages:

- Complex problems/algorithms can be explained with simpler notation
- Can express problems in a form that takes advantage of massive parallelism
- If performed with real chemicals, it drastically reduces the power needed for computation

Disadvantages:

- Electronic real/artificial computation requires a lot of power
    - Although problems may be more scalable given their specifications, they do not scale well in hardware

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Example

Dynamic Neural Network Generation Using Chemical Computation

- Stochastic system, lattice model

Three elements:

- Molecules: cell types - input, neurons, output
- Reactions: allow the cells to communicate
- Dynamics: each grid cell contains different substrates (initial or generated by cells)

Cells communicate via substrates, form/lose connections, reproduce/die

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State of the Art

Quantum Computing: OpenFermion (Google)

- Chemical computation libraries for quantum computing
- Platform for translating conventional code to quantum code
- Open source

Advances in Algorithms

- Time dependent density functional theory measurements – Berkeley labs
- Allow scientists to study the resonant frequency of molecules, which describe its properties and behavior in reactions
- New algorithm reduces the amount of computational resources and time needed by using accurate approximations

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Future Advances

Quantum Computation

- Provides the massive parallelism needed for real and artificial chemical computation
- For real chemical computations, only a few qubits are needed to simulate simple atoms.
- Berkeley Labs – intense research to develop quantum processors, compilers, optimizations, and algorithms specifically targeted at handling chemical computations

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Conclusion / Thank You!

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