ChemLAB

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Chemistry is Fun?

- **Calculate the Charge:**
  
  - \( \text{C}_{169723} \text{H}_{270464} \text{N}_{45688} \text{O}_{52243} \text{S}_9 \text{C}_2 \)

- **Balance:**
  
  - \( \text{K}_3[\text{Fe(SCN)}_6] + \text{Na}_2\text{Cr}_2\text{O}_7 + \text{H}_2\text{SO}_4 \rightarrow \text{Fe(NO}_3)_3 + \text{Cr}_2(\text{SO}_4)_3 + \text{CO}_2 + \text{H}_2\text{O} + \text{Na}_2\text{SO}_4 + \text{KNO}_3 \)
Motivation

– Stoichiometry
– Chemical equilibrium
– Thermodynamics

• Calculations can be extremely tedious once molecules and compounds become complex
## Supported Features

<table>
<thead>
<tr>
<th>Functions</th>
<th>Types</th>
<th>Control/Looping</th>
</tr>
</thead>
<tbody>
<tr>
<td>print</td>
<td>int</td>
<td>if/else</td>
</tr>
<tr>
<td>Balance</td>
<td>String</td>
<td></td>
</tr>
<tr>
<td>mass</td>
<td>double</td>
<td>while</td>
</tr>
<tr>
<td>charge</td>
<td>boolean</td>
<td></td>
</tr>
<tr>
<td>electrons</td>
<td>element</td>
<td>for</td>
</tr>
<tr>
<td>GRAPHICS!!</td>
<td>molecule</td>
<td>return</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operators</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>+ - * / %</td>
<td></td>
</tr>
<tr>
<td>&lt;= == &gt; &gt;= !=</td>
<td></td>
</tr>
<tr>
<td>&amp;&amp;</td>
<td></td>
</tr>
</tbody>
</table>
Architecture

Scanner ➔ Parser ➔ AST ➔ Semantic

Java File ➔ Import Java Library ➔ Java Code ➔ Compiler

Java Compiler ➔ Java Executable!
Language Tutorial

- **MgO + Fe → Fe₂O₃ + Mg**
- **Mg: 1a + 0b + 0c = 1d**
- **Fe: 0a + 1b - 2c = 0d**
- **O: 1a + 0b - 3c = 0d**

Answer: 3MgO + 2Fe → Fe₂O₃ + 3Mg
Language Tutorial

• Syntactic Sugar
  – When you write a graphics function, you don’t need to call it. It will automatically be called!
  – Can concatenate integers and strings – will be converted to a string type
  – Don’t need to specify return types – like python!

• Other Rules
  – Must always declare main function
Language Tutorial

• Built in Functions
  – mol_mass()
  – mol_charge()
  – mol_electrons()
  – balance()
  – draw()
Language Tutorial

// declaring a Simple Hello World
function main()
{
    print "Hello World";
    call message("PLT Rocks!");
}

function message(string x)
{
    print x;
}
function main()
{
    string A;
    element Mg (12,24,2);
    element O (18,16,-2);
    element Fe(26, 56, 3);
    molecule MgO {Mg, O};
    molecule Fe2O3 {Fe, Fe, O, O, O};

    A = balance(MgO, Fe  -->  Fe2O3, Mg);
    print A;
}
// prints 2 Fe  3 MgO --&gt; 3 Mg 1 Fe2O3
function main(){}
function graphics()
{
    draw("K",1,1,1,1,1,1,1,1,0);
    draw("Br",0,0,0,1,0,0,0,0,0);
    draw("Mn",1,1,0,0,0,0,0,0,0);
    draw("O",1,1,1,0,1,1,1,0,0);
    draw("H",1,0,0,0,0,0,0,0,0);
    draw("H",0,1,0,0,0,0,0,0,0);
}
Language Tutorial

• Graphics!
Attempts

• Python – Chemistry Library
• C++ - ChemKit
Proposed Plan

• Everyone does a little of everything
• Biweekly Hangouts
• Weekly Meetings
  – Doodle
  – Paired Programming
  – Slack
Proposed Plan

• Sept 24th: Proposal Due Date
• Oct 2nd: ChemLAB syntax roughly decided upon
• Oct 23th: Scanner/Parser/AST unambiguous and working
• Oct 27th: LRM Due Date
• Nov 9th: Architectural design finalized
• Dec 5th: Compile works, all tests passed
• Dec 12th: Project report and slides completed
• Dec 17th: Final Project Due Date
What Actually Happened...

• Graph of procrastination
Coding Techniques

• Lonely All-Nighter

My eyes hurts...
Need to lower the brightness...

• Cozy Campfire

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Lessons Learned

• Software Dev is more than just coding

• Communication/Planning are the foundation

• Appreciation for how difficult it is to develop a language

• Gained survival skill to trick the heart into thinking everything is going to be alright...in the end!
Demo

- Whoo hoo!
I'd tell you a chemistry joke...

But all the good ones argon.