ChemLAB

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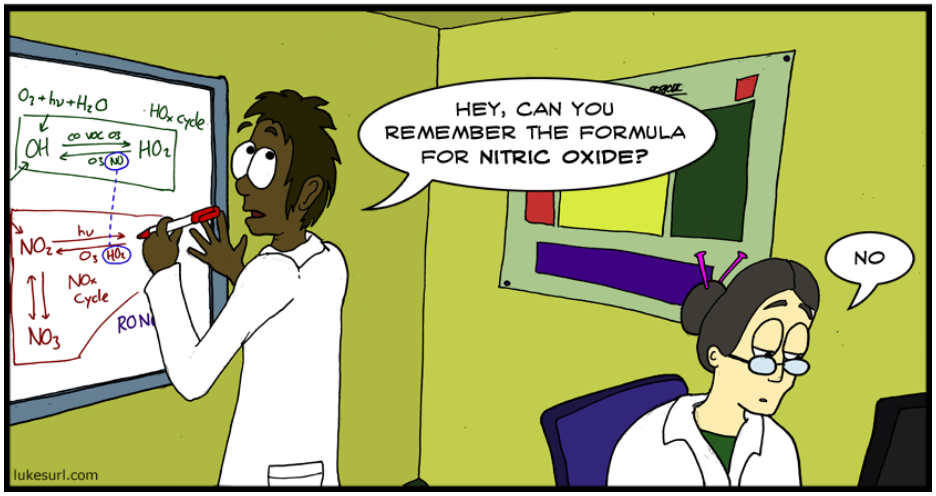
Chemistry is Fun?

- Calculate the Charge:
  - $C_{169723}H_{270464}N_{45688}O_{52243}S_{912}$
- Balance:
  - $K_3[Fe(SCN)_6] + Na_2Cr_2O_7 + H_2SO_4 \rightarrow$

    $Fe(NO_3)_3 + Cr_2(SO_4)_3 + CO_2 + H_2O + Na_2SO_4 + KNO_3$



Motivation

- Stoichiometry
- Chemical equilibrium
- Thermodynamics

- Calculations can be extremely tedious once molecules and compounds become complex

Supported Features

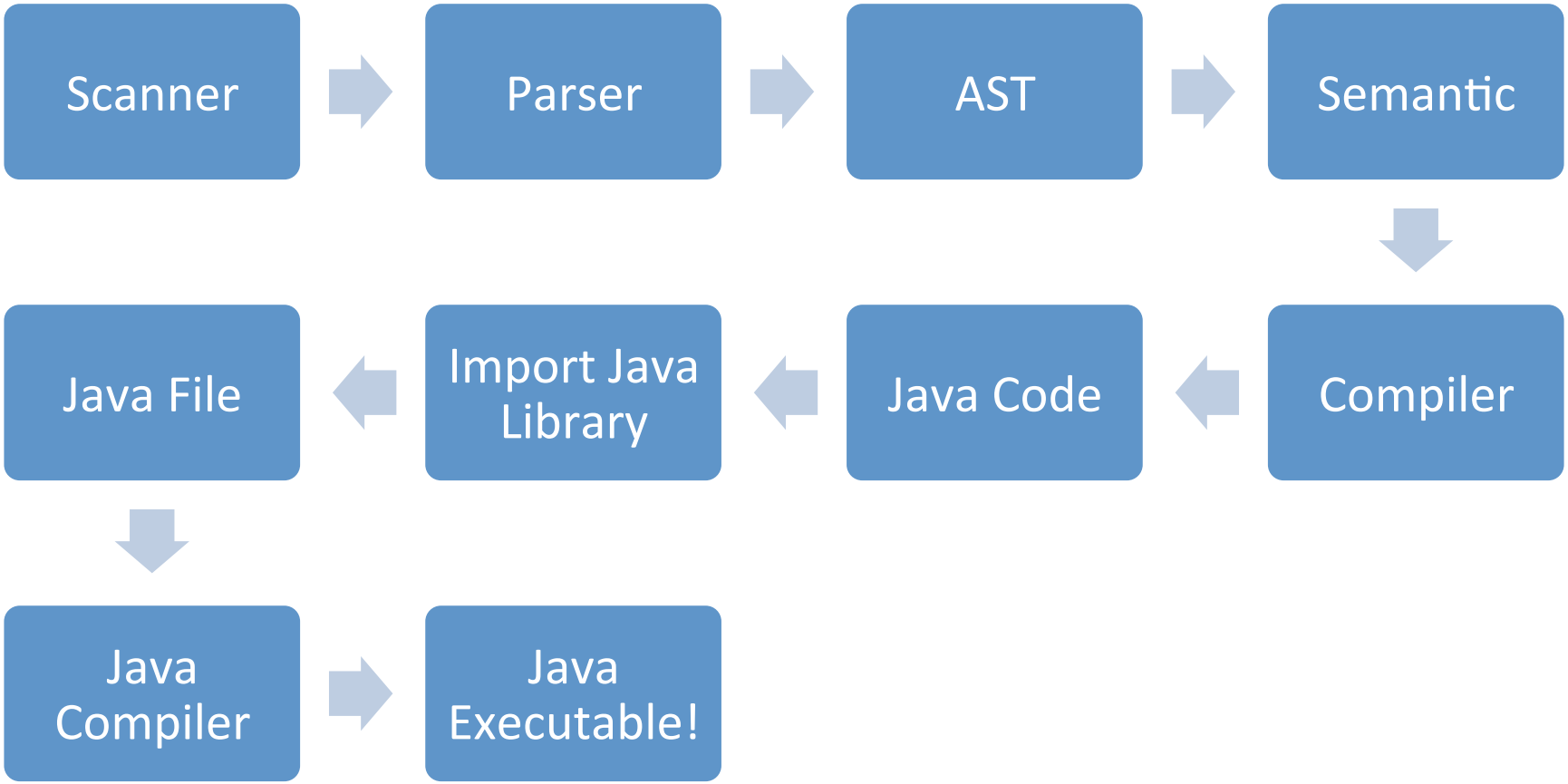
Functions
print
Balance
mass
charge
electrons
GRAPHICS!!!

Operators
+ - * / %
< <= == > >= !=
&& ||

Types
int
String
double
boolean
element
molecule
equation

Control/Looping
if/else
while
for
return

Architecture



Language Tutorial

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

$$A=\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & -2\\ 1 & 0 & 3\end{bmatrix} \quad B=\begin{bmatrix}1\\ 0\\ 0\end{bmatrix}$$

$$\det A=3$$

- Answer: 3MgO + 2Fe —> Fe2O3 + 3Mg

$$[A]^{-1} * [B] * \det[A]=\begin{bmatrix}3\\ 2\\ 1\end{bmatrix}$$

$$a=3,\ b=2,\ c=1,\ d=3$$

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;
}
```

Language Tutorial

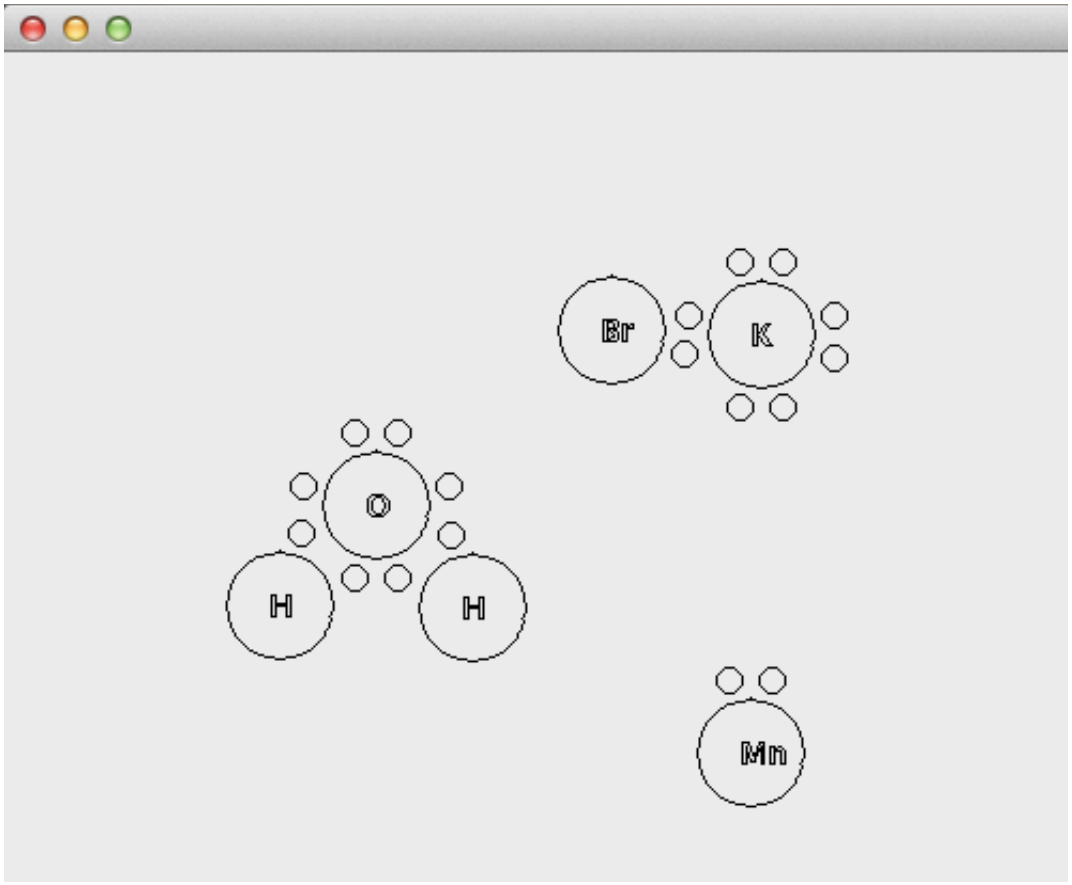
```
function main()
{
        string A;
        element Mg (12,24,2);
        element O (18,16,-2);
        element Fe(26, 56, 3);
        molecule MgO {Mg, O};
        molecule Fe2O3 {Fe, Fe, O, O, O};

        A = balance(MgO, Fe  -->  Fe2O3, Mg);
        print A;
}
// prints 2 Fe  3 MgO --> 3 Mg 1 Fe2O3
```

Language Tutorial

```
function main(){}
function graphics()
{
        draw("K",1,1,1,1,1,1,1,0);
        draw("Br",0,0,0,1,0,0,0,0);
        draw("Mn",1,1,0,0,0,0,0,0);
        draw("O",1,1,1,0,1,1,1,0);
        draw("H",1,0,0,0,0,0,0,0);
        draw("H",0,1,0,0,0,0,0,0);
}
```

Language Tutorial

- Graphics!



Attempts

- Python – Chemistry Library
- C++ - ChemKit

Proposed Plan

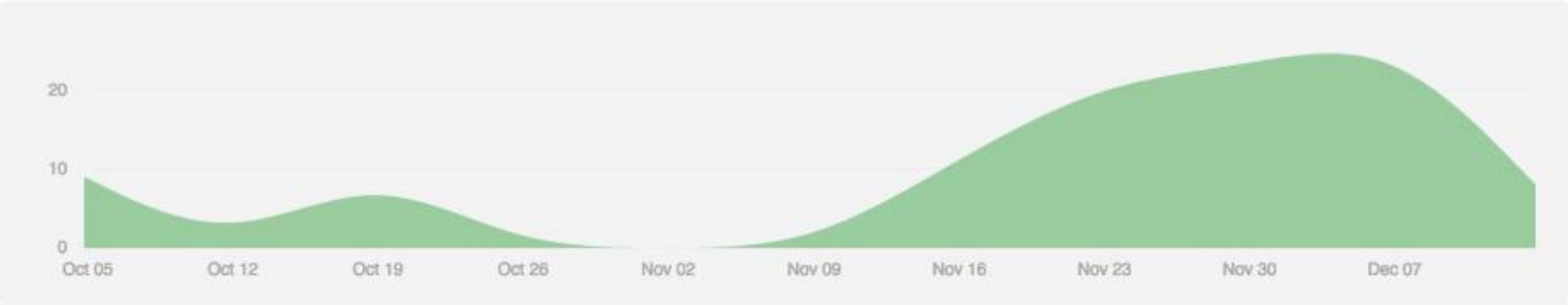
- Everyone does a little of everything
- Biweekly Hangouts
- Weekly Meetings
  - Doodle
  - Paired Programming
  - Slack

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

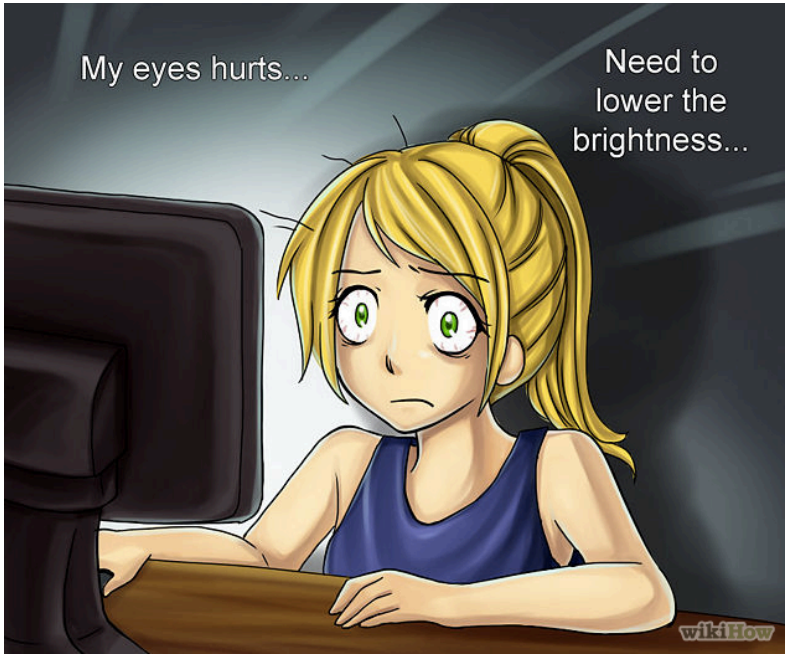
What Actually Happened…

- Graph of procrastination



Coding Techniques

- Lonely All-Nighter



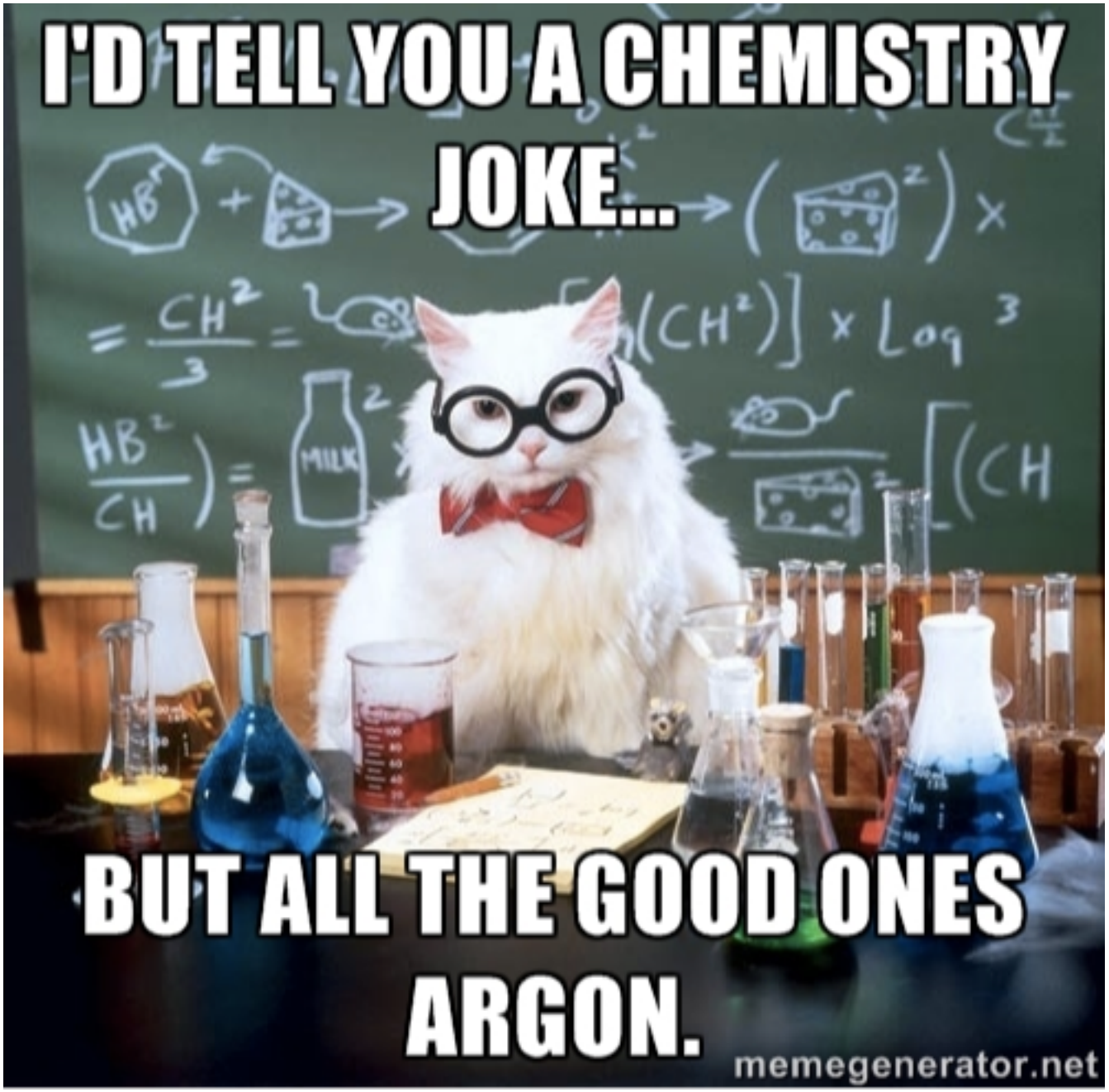
- Cozy Campfire

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!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BUT ALL THE GOOD ONES ARGON.
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