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Going under the hood of MontePy: A python API for MCNP input files

March 2024

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Idaho National Laboratory

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A python API for MCNP input files

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Review of MCNP inputs

- Fortran & Punchcard
- Predates: XML, JSON, SGML
- Very specialized, and pointer based
- Cell example

```
123456      654321      -10.02      -1  2  3  4  imp:n=1.0 imp:p=0.5  fill = 10 ( 0 10.0 20.0)
```

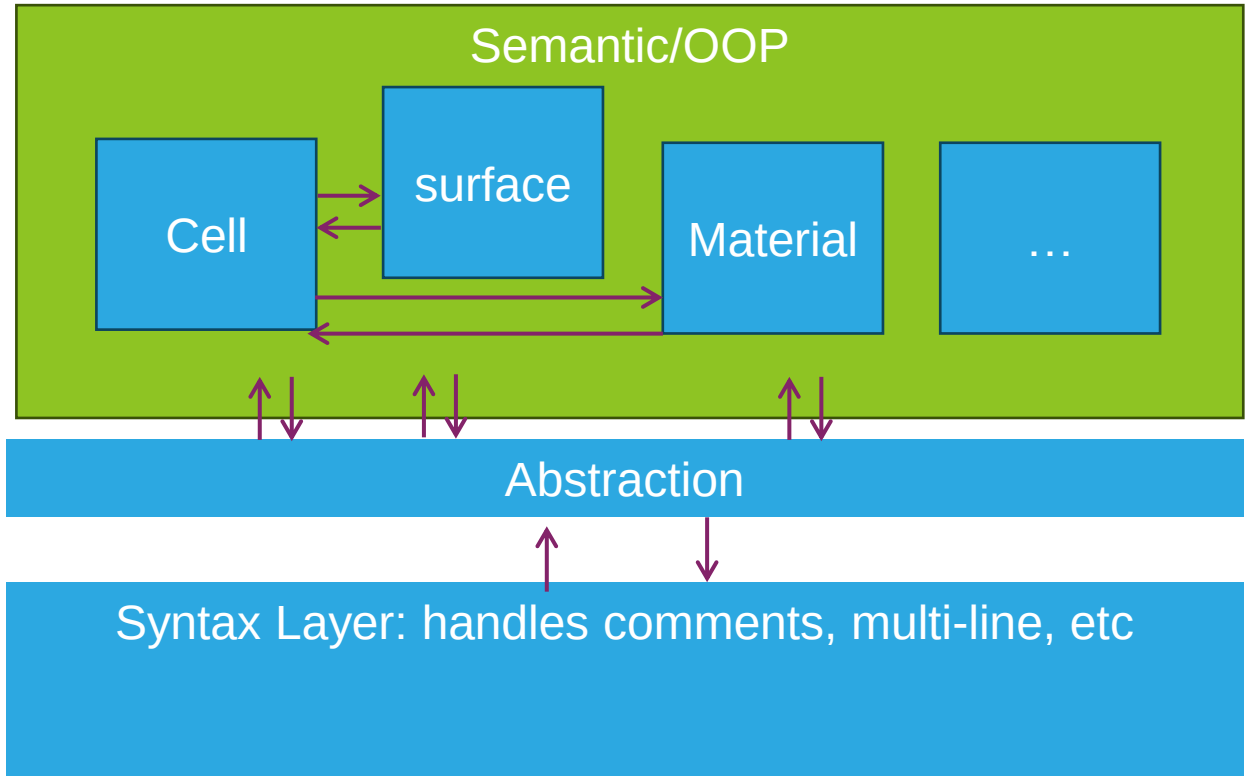
Cell #	mat num	density	geometry	parameters

Problem

- Can’t use standard library (e.g., `import json`)
- Updating pointers can be very tedious
- Finding objects by number is difficult

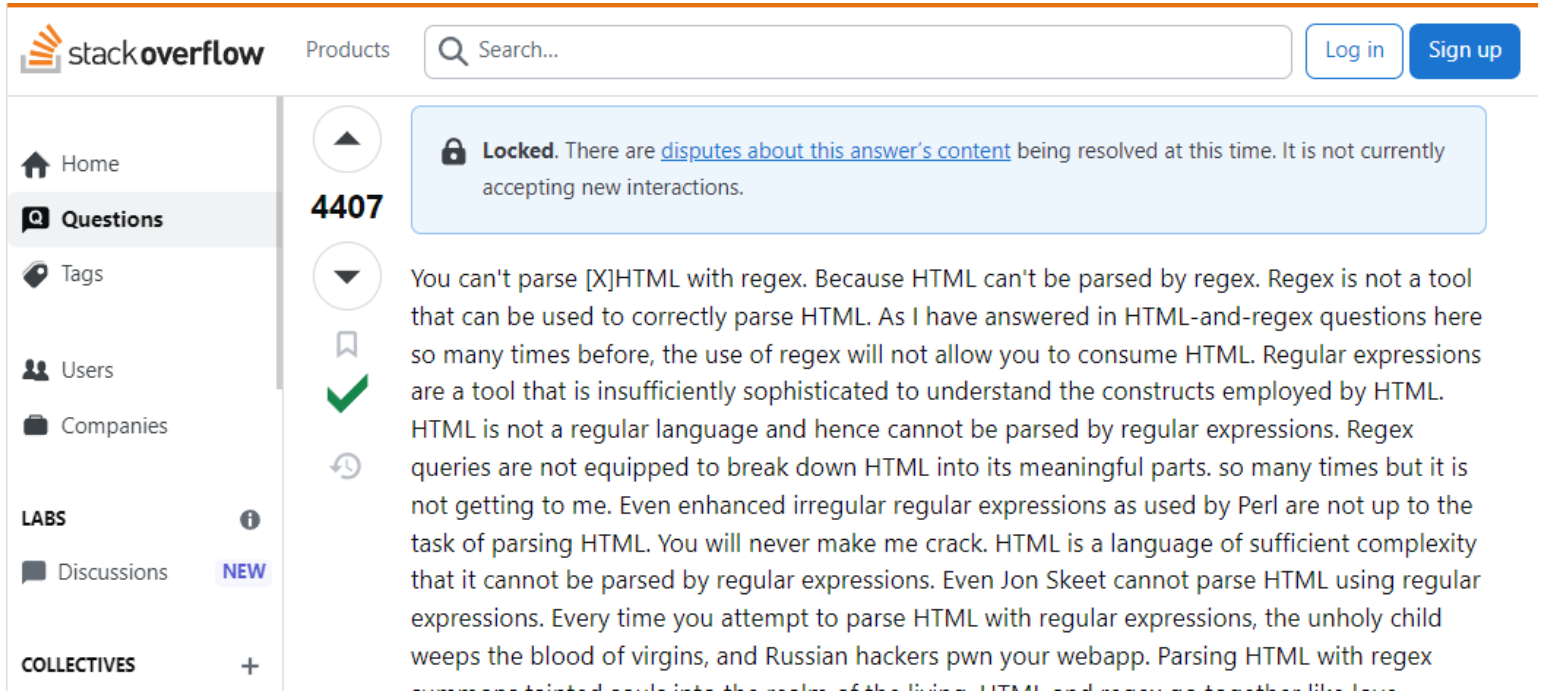
Solution: MontePy

- Object oriented interface



Very Naïve: Regular expressions

- MCNP is not a Regular language!



https://stackoverflow.com/a/1732454

Naïve first attempt: fake parsing (<=0.1.7)

- Handle syntax
- Split on spaces

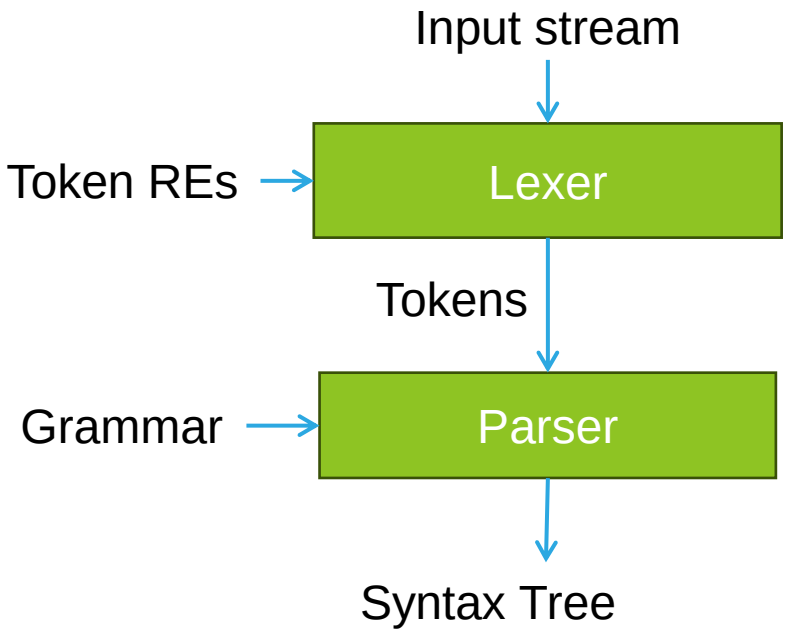
```
123456      654321  -10.02      -1  2  3  4
          imp:n = 1.0 imp:p 0.5
          fill = 10 ( 0 10.0 20.0)
```

```
["123456","654321","-10.02","-1", "2","3","4",
"imp:n","=","1.0","imp:p", "0.5", "fill"…]
```

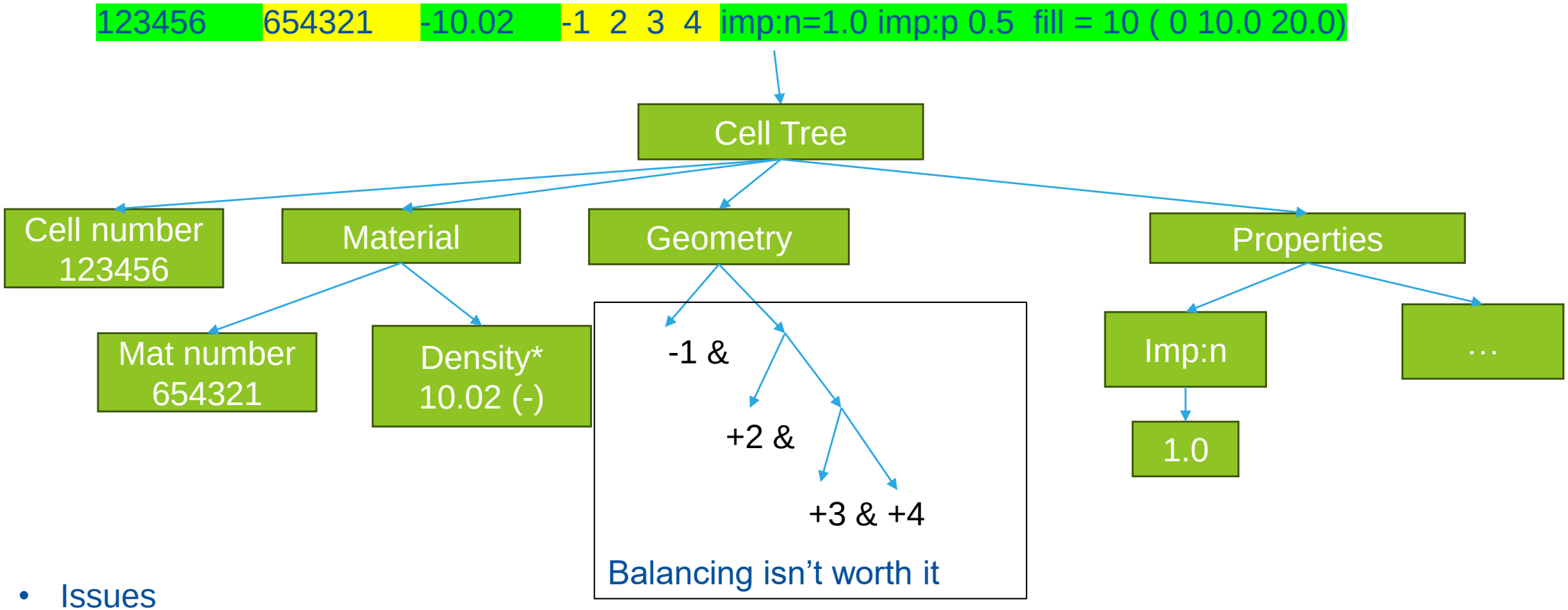
- Lots of formatting reconstruction headaches
- Users actually like their formatting?

Finally doing it right: Lexers Parsers and syntax trees, oh my (>= 0.2.0)

- Requires Context-free grammar
- Uses Lookahead left-to-right (LR) Parser (LALR(1))
- MCNP grammar is contextual
  - Break into context-free chunks
  - Build multiple lexers and parsers



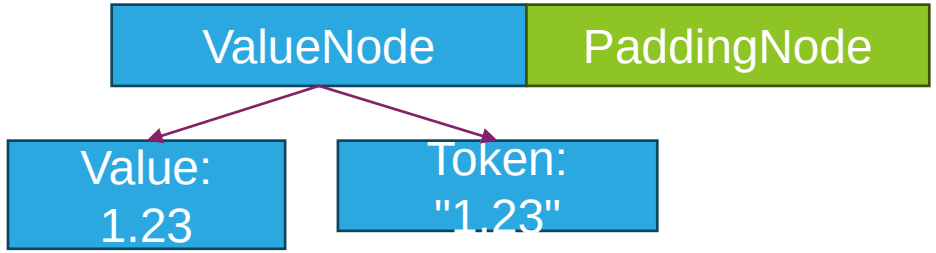
Example Abstract Syntax Tree



- Issues
  - Whitespace is an operator/ implicit operators
  - Users like formatting
    - Need "black", not "python"

Concrete Syntax Trees

- Introduce padding
  - Whitespace + comments
- Glue to leaves



- Reverse Engineering formatting
  - `"10.02 " -> "10.03 "`, *not* `"10.021115 "`
  - `"6.1+23 $ hi" -> "1.0+01 $ hi"`

Everything is an Object, and every variable a pointer

- Objects point to each other
- When possible, properties of objects point to ValueNode
  - When reexported the ValueNode doesn't need to be updated in the syntax tree
  - Everything handled by a decorator to keep it DRY.

```
@make_prop_val_node("_number", int, validator=_number_validator)
def number(self):
    """
    The current cell number that will be written out to a new input.

    :rtype: int
    """
    pass

@make_prop_pointer("_material", (Material, type(None)), deletable=True)
def material(self):
    """
    The Material object for the cell.

    If the material is None this is considered to be voided.

    :rtype: Material
    """
    pass
```

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