Sets and Dictionaries

Nanotech Example

How many molecules of different kinds can we make using the atoms in our warehouse?

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```
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helium : He 1
water : H 2 O 1
hydrogen : H 2
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```
# Atom inventory file

He 1
H 4
O 3
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helium : He 1
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```

```
# Atom inventory file

He 1
H 4
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```

Now have all the tools we need

Natural to represent inventory as dictionary

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Keys: atomic symbols

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Values: number of atoms available

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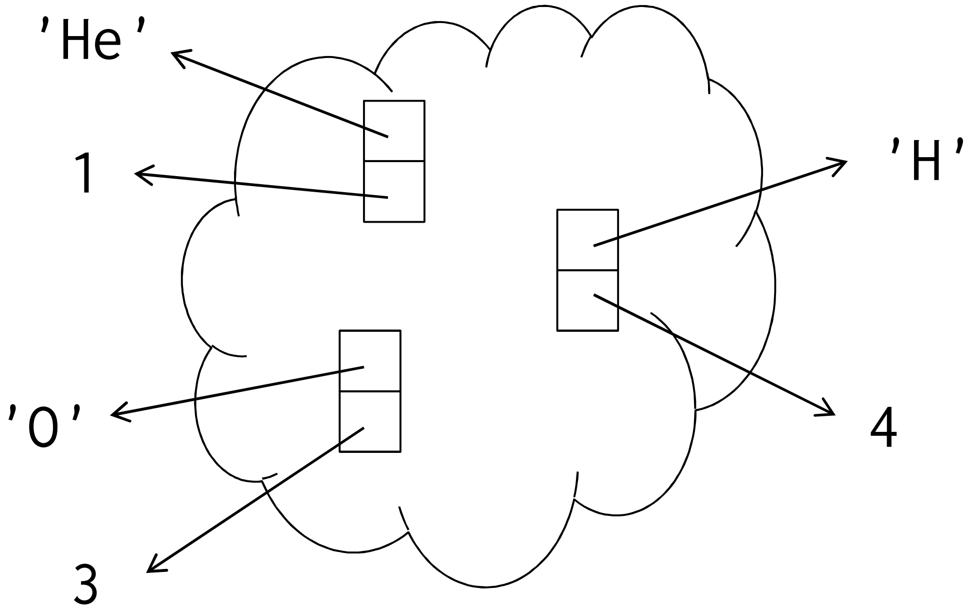

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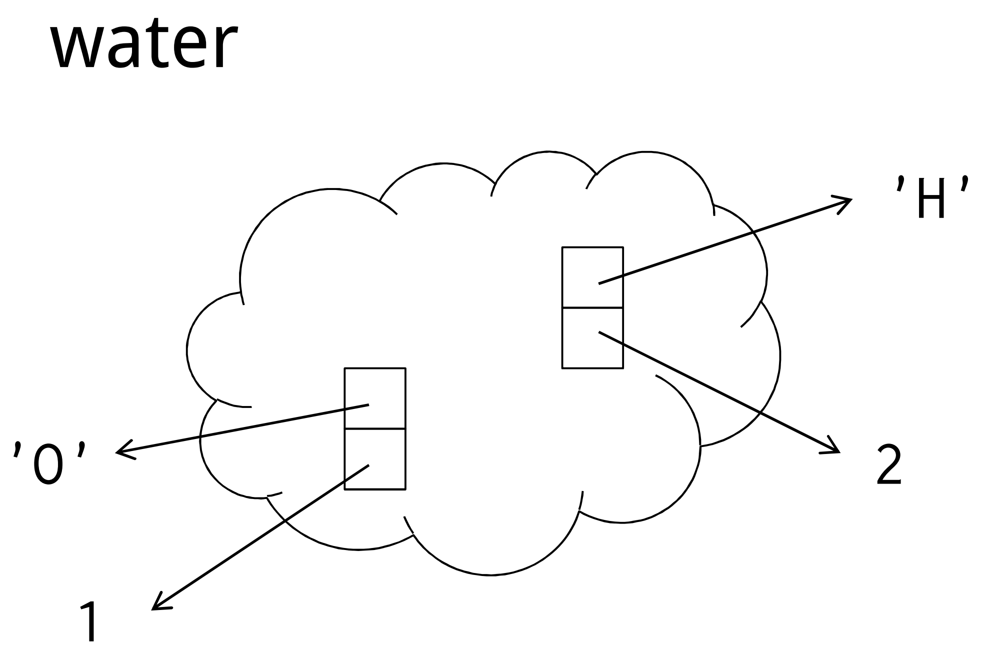

Store formulas as a dictionary of dictionaries

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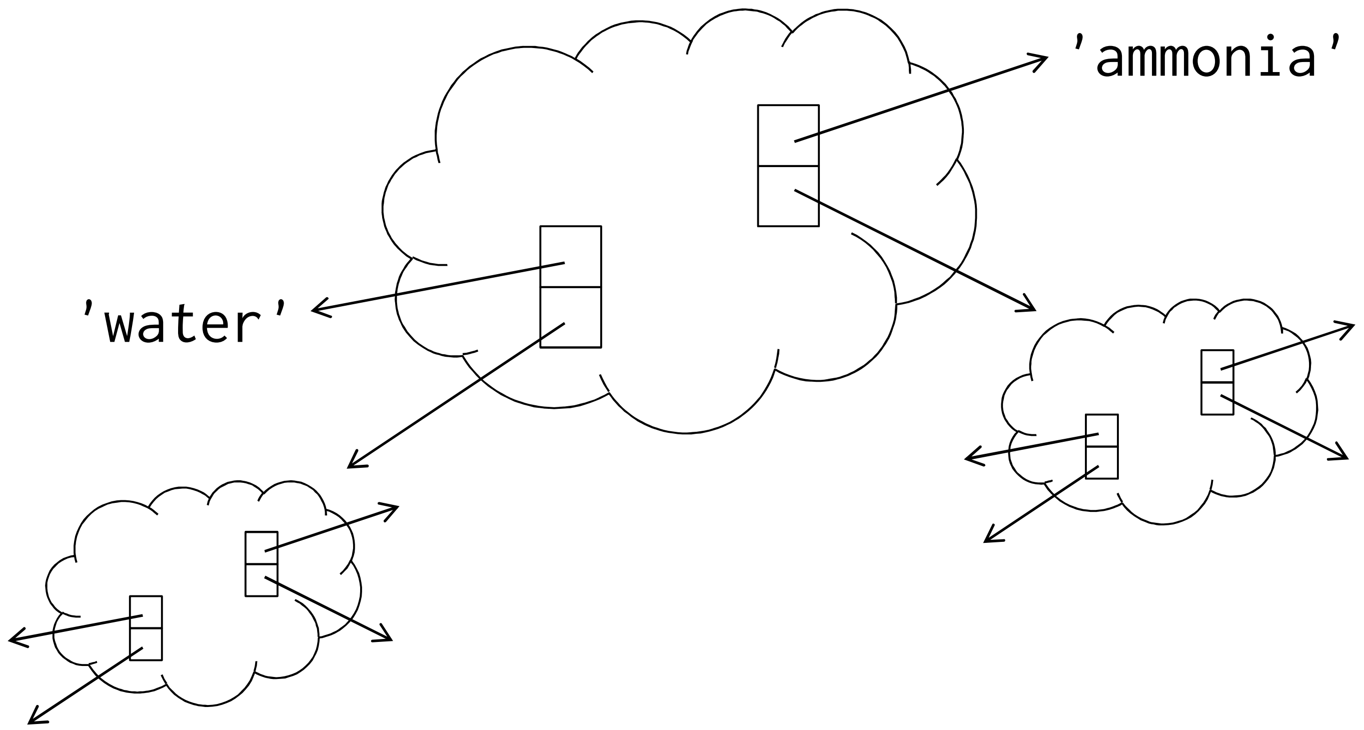

Number of molecules that can be made is:

$$\min_{\text{atom} \in \text{formula}} \frac{\text{available[atom]}}{\text{required[atom]}}$$

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Keys: molecule names

Number of molecules that can be made is:

$$\min_{\text{atom} \in \text{formula}} \frac{\text{available[atom]}}{\text{required[atom]}}$$

If `atom` not in `available`, its count is implicitly 0

Store results in yet another dictionary

Keys: molecule names

Values: counts of how many can be made

```python
'''Calculate how many molecules of each type can be made
with the atoms on hand.'''

import sys

if __name__ == '__main__':
  inventory = read_inventory(sys.argv[1])
  formulas = read_formulas(sys.argv[2])
  counts = calculate_counts(inventory, formulas)
  show_counts(counts)
```

```
def read_inventory(filename):
  '''Read inventory of available atoms.'''

  result = {}
  for line in read_lines(filename):
    name, count = line.split(' ')
    result[name] = int(count)

  return result
```

```
def read_lines(filename):
  '''Read lines from file, stripping out
  blank lines and comments.'''

  reader = open(filename, 'r')
  lines = []
  for line in reader:
    line = line.split('#')[0].strip()
    if line:
      lines.append(line)
  reader.close()

  return lines
```

```
def read_formulas(filename):
  '''Read molecular formulas from file.'''

  result = {}
  for line in read_lines(filename):

    name, atoms = line.split(':')
    name = name.strip()

    atoms = atoms.strip().split(' ')
    formula = {}
    for i in range(0, len(atoms), 2):
      formula[atoms[i]] = int(atoms[i+1])

    result[name] = formula

  return result
```

```
def read_formulas(filename):
  '''Read molecular formulas from file.'''

  result = {}
  for line in read_lines(filename):

    name, atoms = line.split(':')
    name = name.strip()

    atoms = atoms.strip().split(' ')
    formula = {}
    for i in range(0, len(atoms), 2):
      formula[atoms[i]] = int(atoms[i+1])

    result[name] = formula

  return result
```

Storing results in dictionary

```
def read_formulas(filename):
  '''Read molecular formulas from file.'''

  result = {}
  for line in read_lines(filename):

    name, atoms = line.split(':')
    name = name.strip()

    atoms = atoms.strip().split(' ')
    formula = {}
    for i in range(0, len(atoms), 2):
      formula[atoms[i]] = int(atoms[i+1])

    result[name] = formula

  return result
```

$\leftarrow$ For each interesting line in the input file...

```
def read_formulas(filename):
  '''Read molecular formulas from file.'''

  result = {}
  for line in read_lines(filename):

    name, atoms = line.split(':')
    name = name.strip()

    atoms = atoms.strip().split(' ')
    formula = {}
    for i in range(0, len(atoms), 2):
      formula[atoms[i]] = int(atoms[i+1])

    result[name] = formula

  return result
```

$\leftarrow$ Separate the molecule name and the formula

```
def read_formulas(filename):
  '''Read molecular formulas from file.'''

  result = {}
  for line in read_lines(filename):

    name, atoms = line.split(':')
    name = name.strip()

    atoms = atoms.strip().split(' ')
    formula = {}
    for i in range(0, len(atoms), 2):
      formula[atoms[i]] = int(atoms[i+1])

    result[name] = formula

  return result
```

Separate the atoms and their counts

```
def read_formulas(filename):
  '''Read molecular formulas from file.'''

  result = {}
  for line in read_lines(filename):

    name, atoms = line.split(':')
    name = name.strip()

    atoms = atoms.strip().split(' ')
    formula = {}
    for i in range(0, len(atoms), 2):
      formula[atoms[i]] = int(atoms[i+1])

    result[name] = formula

  return result
```

Loop over pairs of atoms and counts

```
def read_formulas(filename):
  '''Read molecular formulas from file.'''

  result = {}
  for line in read_lines(filename):

    name, atoms = line.split(':')
    name = name.strip()

    atoms = atoms.strip().split(' ')
    formula = {}
    for i in range(0, len(atoms), 2):
      formula[atoms[i]] = int(atoms[i+1])

    result[name] = formula

  return result
```

Store the count as an integer with the atomic symbol as key

```
def read_formulas(filename):
  '''Read molecular formulas from file.'''

  result = {}
  for line in read_lines(filename):

    name, atoms = line.split(':')
    name = name.strip()

    atoms = atoms.strip().split(' ')
    formula = {}
    for i in range(0, len(atoms), 2):
      formula[atoms[i]] = int(atoms[i+1])

    result[name] = formula

  return result
```

And store the molecule in the main dictionary

```
def calculate_counts(inventory, formulas):
  '''Calculate how many of each molecule
  can be made with inventory.'''

  counts = {}
  for name in formulas:
    counts[name] = dict_divide(inventory,
                               formulas[name])

  return counts
```

```
def calculate_counts(inventory, formulas):
  '''Calculate how many of each molecule
  can be made with inventory.'''

  counts = {}
  for name in formulas:
    counts[name] = dict_divide(inventory,
                                  formulas[name])

  return counts
```

Sub-dictionary holding atom counts for a particular molecule

```
def calculate_counts(inventory, formulas):
  '''Calculate how many of each molecule
  can be made with inventory.'''

  counts = {}
  for name in formulas:
    counts[name] = dict_divide(inventory,
                               formulas[name])

  return counts
```

Big functions: nothing is obviously wrong

```
def calculate_counts(inventory, formulas):
  '''Calculate how many of each molecule
  can be made with inventory.'''

  counts = {}
  for name in formulas:
    counts[name] = dict_divide(inventory,
                               formulas[name])

  return counts
```

Big functions: nothing is obviously wrong

Small functions: obviously, nothing is wrong

```
def dict_divide(inventory, molecule):
  '''Calculate how much of a single molecule
  can be made with inventory.'''

  number = None
  for atom in molecule:
    required = molecule[atom]
    available = inventory.get(atom, 0)
    limit = available / required
    if (number is None) or (limit < number):
      number = limit

  return number
```

```
def dict_divide(inventory, molecule):
  '''Calculate how much of a single molecule
  can be made with inventory.'''

  number = None
  for atom in molecule:
    required = molecule[atom]
    available = inventory.get(atom, 0)
    limit = available / required
    if (number is None) or (limit < number):
      number = limit

  return number
```

Identical format:

keys are atoms,

values are counts

```
def dict_divide(inventory, molecule):
  '''Calculate how much of a single molecule
  can be made with inventory.'''

  number = None
  for atom in molecule:
    required = molecule[atom]
    available = inventory.get(atom, 0)
    limit = available / required
    if (number is None) or (limit < number):
      number = limit

  return number
```

Common pattern: None means "uninitialized", so initialize the first time through the loop

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def dict_divide(inventory, molecule):
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  can be made with inventory.'''

  number = None
  for atom in molecule:
    required = molecule[atom]
    available = inventory.get(atom, 0)
    limit = available / required
    if (number is None) or (limit < number):
      number = limit

  return number
```

Common pattern:

stored value or default

```
def dict_divide(inventory, molecule):
  '''Calculate how much of a single molecule
  can be made with inventory.'''

  number = None
  for atom in molecule:
    required = molecule[atom]
    available = inventory.get(atom, 0)
    limit = available / required
    if (number is None) or (limit < number):
      number = limit

  return number
```

Common pattern:

find minimum of

calculated values

```
def show_counts(counts):
  '''Show how many of each molecule can be made.'''

  counts = invert_dict(counts)
  for key in sorted(counts.keys(), reverse=True):
    for name in sorted(counts[key]):
      print key, name
```

```
def show_counts(counts):
  '''Show how many of each molecule can be made.'''

  counts = invert_dict(counts)
  for key in sorted(counts.keys(), reverse=True):
    for name in sorted(counts[key]):
      print key, name
```

Reverse to get greatest first

```
def invert_dict(src):
  '''Invert a dictionary, returning value->set{key}.'''

  dst = {}
  for key in src:
    value = src[key]
    if value not in dst:
      dst[value] = set()
    dst[value].add(key)

  return dst
```

```
def invert_dict(src):
  '''Invert a dictionary, returning value->set{key}.'''

  dst = {}
  for key in src:
    value = src[key]
    if value not in dst:
      dst[value] = set()
    dst[value].add(key)

  return dst
```

Common pattern:
make sure there's a
collection, then add

```
def show_counts(counts):
  '''Show how many of each molecule can be made.'''

  counts = invert_dict(counts)
  for key in sorted(counts.keys(), reverse=True):
    if key > 0:
      for name in sorted(counts[key]):
        print key, name
```

Go back and only show molecules that can actually be made

```
# inventory-00.txt
```

```
# formulas-01.txt

helium : He 1
```

No output, which is correct.

```
# inventory-01.txt
He 1
```

```
# formulas-01.txt

helium : He 1
```

1 helium

```
# inventory-02.txt
He 1
H 4
```

```
# formulas-01.txt

helium : He 1
```

```
1 helium
```

```
# inventory-02.txt
He 1
H 4
```

```
# formulas-02.txt

helium : He 1
water : H 2 O 1
```

```
1 helium
```

```
# inventory-02.txt
He 1
H 4
```

```
# formulas-03.txt

helium : He 1
water : H 2 O 1
hydrogen : H 2
```

2 hydrogen

1 helium

```
# inventory-03.txt
He 1
H 4
O 3
```

```
# formulas-03.txt

helium : He 1
water : H 2 O 1
hydrogen : H 2
```

2 hydrogen

2 water

1 helium

```
# inventory-03.txt
He 1
H 4
O 3
```

```
# formulas-03.txt

helium : He 1
water : H 2 O 1
hydrogen : H 2
```

```
2 hydrogen

2 water

1 helium
```

Looks good...

```
# inventory-03.txt
He 1
H 4
O 3
```

```
# formulas-03.txt

helium : He 1
water : H 2 O 1
hydrogen : H 2
```

```
2 hydrogen

2 water

1 helium
```

Looks good...

Code is *much* simpler than it would be using lists of pairs created by

Greg Wilson

June 2010