Constructing Scientific Programs with SymPy

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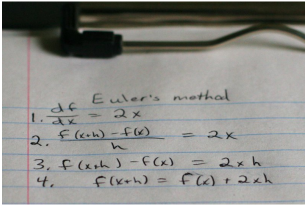
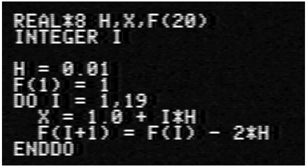
Outline

Writing Scientific Programs by Hand

Derive equations

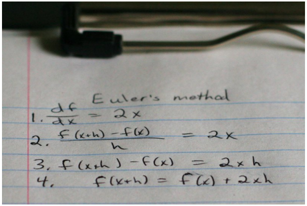


Convert to code



Writing Scientific Programs by Hand

Derive equations



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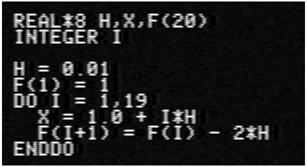


Problems:

- Transcription errors
- Identifying error from testing final program

How Should We Write Scientific Programs?

Any problem in computer science can be solved with another layer of indirection.

David Wheeler

I'd rather write programs to write programs than write programs

Richard Sites

Computational Thinking - The thought processes involved in formulating problems so their solutions can be represented as computational steps and algorithms.

Alfred Aho

Components of a Program to Write Scientific Programs

- Description of problem
  - Domain Specific Language
  - Symbolic mathematics
- Transformation to target
- Representation of target language/system

Other Projects

- FEniCS - Finite element solutions to differential equations
- SAGA (Scientific computing with Algebraic and Generative Abstractions) - PDE’s
- Spiral - signal processing transforms
- TCE (Tensor Contraction Engine) - quantum chemistry
- FLAME (Formal Linear Algebra Method Environment) - Linear algebra

See Andy Terrel’s article in CiSE March/April 2011

Advantages and Disadvantages

- Advantages
  - Improved notation for expressing problems and algorithms
  - Testability - transforms are 'ordinary software'
  - Optimization of generated code
    - Domain specific optimizations
    - Explore larger parameter space
    - Restructuring for various target systems
- Disadvantages
  - If problem domain isn't covered by existing project, ?

Outline

Motivation and Overview of Writing Scientific Programs

Implementation of a Framework

Example: Partition Function Integral

Implementing Components of a Program to Write Scientific Programs

- Description of problem
  - Symbolic mathematics - SymPy expressions
  - Structure above expressions - derivation modeling
- Transformation to target - pattern matching
- Representation of target language/system - classes for C++ and Python

Derivation Modeling - What is it?

Think of math homework

- Series of steps
- Show your work

Solve for x:

$$\begin{aligned} 2x + y &= 44 \\ 2x &= 44 - y \\ x &= 22 - y/2 \end{aligned}$$

Types of steps

- Exact transformations
- Approximations
- Specialization - no. of spatial dimensions, no. of particles

Derivation Modeling

`derivation` class

- constructor takes initial equation
- `add_step`
- `final` or `new_derivation`

Examples of steps:

- replace
- add_term
- specialize_integral

Also outputs steps to web page in MathML or MathJax for nicely rendered math.

Derivation Modeling - Example

```
from sympy import Symbol,S
from prototype.derivation import \
    derivation, add_term, mul_factor

x,y = Symbol('x'),Symbol('y')
d = derivation(2*x+y,44)
d.add_step(add_term(-y),'Subtract y')
d.add_step(mul_factor(S.Half),'Divide by 2')
print d.final()
```

Output:

```
x == -y/2 + 22
```

Transform to Target System - Pattern Matching

```python
from sympy import Symbol, print_tree
x,y = Symbol('x'), Symbol('y')
e = x+y
print_tree(e)
```

```
Add: x + y
+-Symbol: y
| comparable: False
+-Symbol: x
  comparable: False
```

Transform to Target System - Pattern Matching

```
Add: x + y
+-Symbol: y
| comparable: False
+-Symbol: x
  comparable: False
```

Match SymPy expression in Python

```python
v = AutoVar()
m = Match(e)
if m(Add, v.e1, v.e2):
    # operate on v.e1 and v.e2
```

Transform to Target System - Pattern Matching 2

`object.__getattr__(self,name)`
If attribute not found, this method is called

```
class AutoVar(object):
    def __init__(self):
        self.vars = []
    def __getattr__(self,name):
        self.vars.append(name)
        return AutoVarInstance(self,name)
```

Transform to Target System - Pattern Matching 3

```
def expr_to_py(e):
  v = AutoVar()
  m = Match(e)
  # subtraction
  if m(Add, (Mul, S.NegativeOne, v.e1), v.e2):
    return py_expr(py_expr.PY_OP_MINUS, expr_to_py(v.e2),
                   expr_to_py(v.e1))
  # addition
  if m(Add, v.e1, v.e2):
    return py_expr(py_expr.PY_OP_PLUS, expr_to_py(v.e1),
                   expr_to_py(v.e2))
  # division
  if m(Mul, v.e1, (Pow, v.e2, S.NegativeOne)):
    return py_expr(py_expr.PY_OP_DIVIDE, expr_to_py(v.e1)
                   expr_to_py(v.e2))
```

Approaches to Code Generation

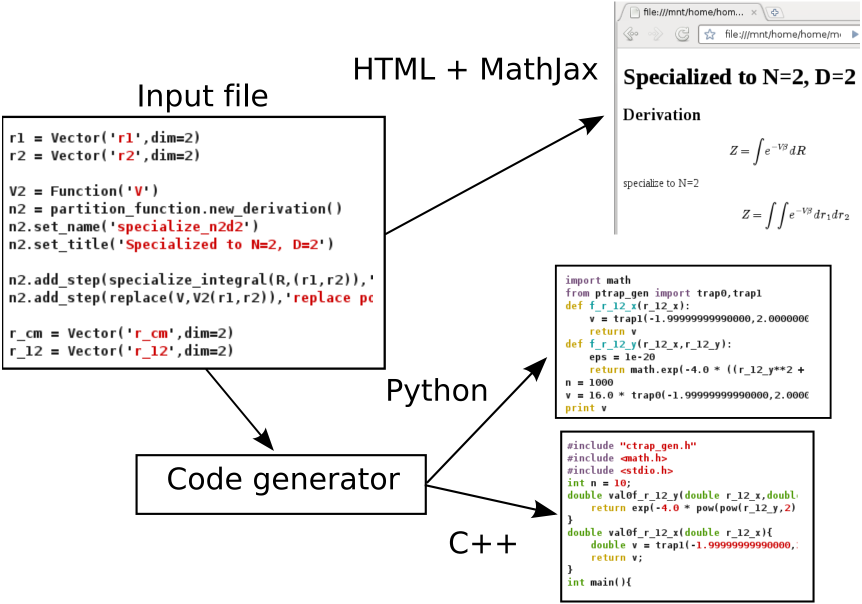
- Print target as string

```
print "print 'Hello' "
```

- General (text-based) templating
- Structured model of target language and system

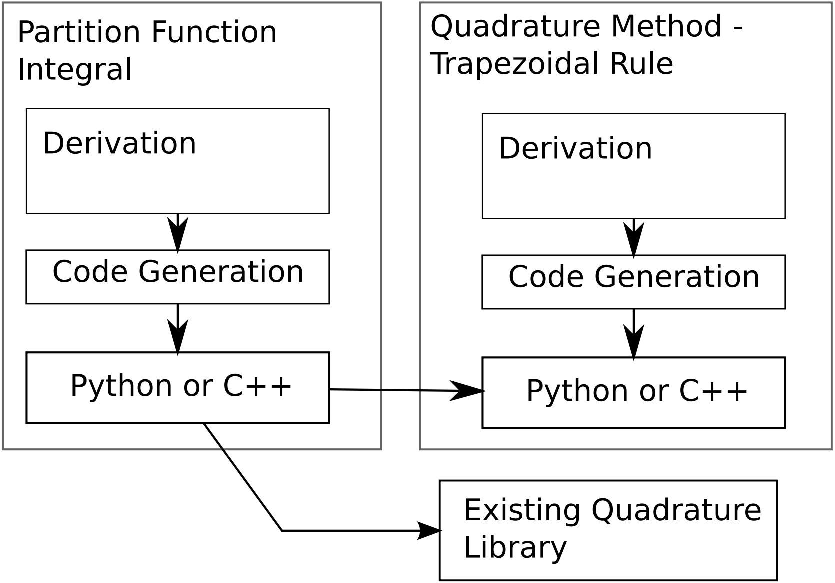
```
py_print_stmt(py_string("Hello"))
```

Overview of workflow



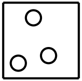
Outline

Example from Statistical Mechanics



Example from Statistical Mechanics

Partition function describes thermodynamics of a system



```
Z = Symbol('Z')
partition_function =
    derivation(Z,Integral(exp(-V/(k*T)),R))
```

$$Z = \int e^{-\frac{V}{Tk}}\, dR$$

Example from Statistical Mechanics 2

```
n2.add_step(specialize_integral(R,(r1,r2)),
    "specialize to N=2")
n2.add_step(replace(V,V2(r1,r2)),
    "replace potential with N=2")
```

$$Z = \int \int e^{-\beta \mathrm{V}(r_1, r_2)} \, dr_1 dr_2$$

Example from Statistical Mechanics 3

```
r_cm = Vector('r_cm',dim=2)
r_12 = Vector('r_12',dim=2)
r_12_def = definition(r_12, r2-r1)
r_cm_def = definition(r_cm, (r1+r2)/2)
V12 = Function('V')
n2.add_step(specialize_integral(r1,(r_12,r_cm)),
    'Switch variables')
n2.add_step(replace(V2(r1,r2),V12(r_12)),
    'Specialize to a potential that depends only on inter
n2.add_step(replace(V12(r_12),V12(Abs(r_12))),
    'Depend only on the magnitude of the distance')
```

$$Z = \int \int e^{-\beta \mathrm{V}(r_{12})} dr_{12} dr_{cm}$$

Example from Statistical Mechanics 4

Integrate out r_{cm}, decompose into vector components and add integration limits

$$Z = L^2 \int_{-\frac{1}{2}L}^{\frac{1}{2}L} \int_{-\frac{1}{2}L}^{\frac{1}{2}L} e^{-\beta \, \mathsf{V}(r_{12x}, r_{12y})} \, dr_{12x} dr_{12y}$$

Example from Statistical Mechanics 5

Specialize to Lennard-Jones potential.

$$\mathrm{V}\left(r\right) = -\frac{4}{r^{6}} + \frac{4}{r^{12}} \tag{1}$$

Insert values for box size, and temperature

$$Z = 16.0 \int_{-2.0}^{2.0} \int_{-2.0}^{2.0} e^{4.0 \frac{1}{\left(r_{12x}^{2} + r_{12y}^{2}\right)^{3}} - 4.0 \frac{1}{\left(r_{12x}^{2} + r_{12y}^{2}\right)^{6}}} \, dr_{12x} dr_{12y}$$

Results

Method	Value	Time (seconds)
`scipy.integrate.dblquad`	285.97597	0.4
Trapezoidal rule (N=1000)	285.97594	
Python		2.9
Shedskin (Python -> C++)		0.5
C++		0.5

Summary

More information at

`http://quantum_mc.blogspot.com`

Code available on GitHub

`https://github.com/markdewing/sympy/tree/`
`derivation_modeling/sympy/prototype`

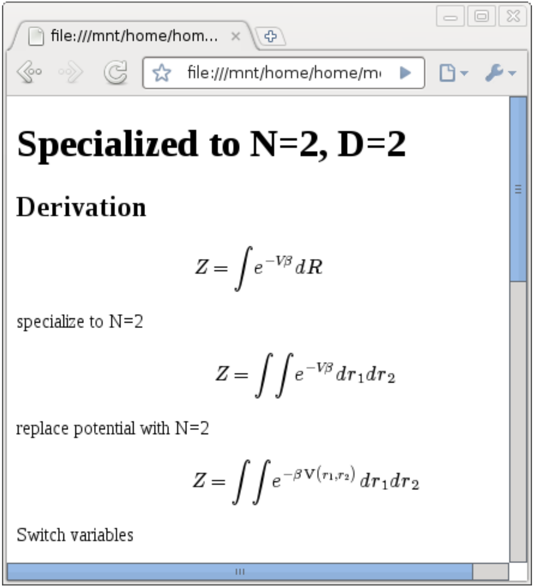
Backup

Input file

File Edit View Terminal Help

```
from sympy import Symbol, Integral, exp, Function, Abs, Eq
from sympy.prototype.vector import Vector, VectorMagnitude
from sympy.prototype.vector_utils import decompose, add_limits, replace_func
from sympy.prototype.derivation import derivation, definition, replace_definition, specialize_integral, replace, do_integral, identity
from partition import partition_function, beta_def, R, V

r1 = Vector('r1',dim=2)
r2 = Vector('r2',dim=2)

V2 = Function('V')
n2 = partition_function.new_derivation()
n2.set_name('specialize_n2d2')
n2.set_title('Specialized to N=2, D=2')

n2.add_step(specialize_integral(R,(r1,r2)),'specialize to N=2')
n2.add_step(replace(V,V2(r1,r2)),'replace potential with N=2')

r_cm = Vector('r_cm',dim=2)
r_12 = Vector('r_12',dim=2)

r_12_def = definition(r_12, r2-r1)
r_cm_def = definition(r_cm, (r1+r2)/2)

V12 = Function('V')

                                                  29,0-1          16%
```

Output - HTML + MathJax



Specialized to N=2, D=2

Derivation

$$Z = \int e^{-V\beta} dR$$

specialize to N=2

$$Z = \int \int e^{-V\beta} dr_1 dr_2$$

replace potential with N=2

$$Z = \int \int e^{-\beta \mathrm{V}(r_1, r_2)} dr_1 dr_2$$

Switch variables

Code generation output - Python

File Edit View Terminal Help

```
import math
from ptrap_gen import trap0,trap1
def f_r_12_x(r_12_x):
    v = trap1(-1.99999999990000,2.00000000000000,f_r_12_y,n,r_12_x)
    return v
def f_r_12_y(r_12_x,r_12_y):
    eps = 1e-20
    return math.exp(-4.0 * ((r_12_y**2 + r_12_x**2 +eps)**-6) + 4.0 * ((
r_12_y**2 + r_12_x**2 +eps)**-3))
n = 1000
v = 16.0 * trap0(-1.99999999990000,2.00000000000000,f_r_12_x,n)
print v

~
~
                                                            12,0-1        All
```

Code generation output - C++

File Edit View Terminal Help

```
#include "ctrap_gen.h"
#include <math.h>
#include <stdio.h>
int n = 10;
double valOf_r_12_y(double r_12_x,double r_12_y){
    return exp(-4.0 * pow(pow(r_12_y,2) + pow(r_12_x,2),-6) + 4.0 * pow(
pow(r_12_y,2) + pow(r_12_x,2),-3));
}
double valOf_r_12_x(double r_12_x){
    double v = trap1(-1.99999999990000,2.00000000000000,valOf_r_12_y,n,r
_12_x);
    return v;
}
int main(){
    double val0 = trap0(-1.99999999990000,2.00000000000000,valOf_r_12_x,
n);
    double v = 16.0 * val0;
    printf("val = %g\n",v);
    return 0;
}

                                                    18,0-1         All
```