High-Level Parallel Programming

1. High-Level Parallel Programming
   - models and tools
2. Multiprocessing in Python
   - scripting in computational science
   - the multiprocessing module
   - numerical integration with multiple processes
3. Multithreading with Julia
   - a fresh approach to numerical computing
   - parallel matrix matrix multiplication
   - parallel numerical integration

MCS 572 Lecture 3
Introduction to Supercomputing
Jan Verschelde, 30 August 2024

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high-level parallel programming

What is high-level parallel programming?

Some characteristics:

- familiar: no new language needed,
- interactive: quick feedback,
- personal: no supercomputer.

Rapid prototyping can decide if parallelism is feasible for a particular computation in an application.

the HLPP conference series

The 17th international symposium on High-Level Parallel Programming and Applications (HLPP 2024), was held in Pisa, Italy, July 4-5, 2024.

Some of the topics include

- high-level programming and performance models,
- software synthesis, automatic code generation,
- applications using high-level languages and tools,
- formal models of verification.

While “high-level” also covers abstract and formal,
there is a need for practical software and tools,
so the “high-level” is not the opposite of technical.

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computations with Python

Advantages of the scripting language Python:

- educational, good for novice programmers;
- packages for scientific computing: NumPy, SciPy, SymPy.

SageMath, a free open source mathematics software system, uses Python to interface many open source software packages.

Our example: $\displaystyle \int_0^1 \sqrt{1-x^2}dx = \frac{\pi}{4}$.

We will use the Simpson rule (available in `SciPy`) as a relatively computational intensive example.

interactive computing

In a Powershell window:

```
Python 3.10.1 (tags/v3.10.1:2cd268a, Dec  6 2021,
19:10:37) MSC v.1929 64 bit (AMD64)] on win32
Type "help", "copyright", "credits" or "license"
for more information.
>>> from scipy.integrate import simps
>>> from numpy import linspace
>>> from numpy.lib.scimath import sqrt
>>> f = lambda x: sqrt(1-x**2)
>>> r = linspace(0,1,1000)
>>> y = f(r)
>>> I = simps(y,r)
>>> 4*I
3.141570366671104
>>>
```

the script simpson4pi.py

```
from scipy.integrate import simps
from numpy import linspace, pi
from numpy.lib.scimath import sqrt

f = lambda x: sqrt(1-x**2)

for k in range(2,9):
    x = linspace(0,1,10**k);
    y = f(x);
    I = 4*simps(y,x)
    print('10^%d' % k, \
          '%.16e' % I, \
          '%.2e' % abs(I - pi))
```

running the script `simpson4pi.py`

The output on screen:

```
10^2 3.140876361334828e+00 7.16e-04
10^3 3.1415703366671104e+00 2.23e-05
10^4 3.141591948898189e+00 7.05e-07
10^5 3.1415926313087348e+00 2.23e-08
10^6 3.1415926528852145e+00 7.05e-10
10^7 3.1415926535675127e+00 2.23e-11
10^8 3.1415926535890946e+00 6.99e-13
```

Getting the execution times:

- on Linux and Mac: `time python simpson4pi.py`
- on Windows: `Measure-Command {python simpson4pi.py}`

timing on Windows

```
Measure-Command {python simpson4pi.py}

Days              : 0
Hours             : 0
Minutes           : 0
Seconds           : 5
Milliseconds      : 785
Ticks             : 57852572
TotalDays         : 6.69589953703704E-05
TotalHours        : 0.00160701588888889
TotalMinutes      : 0.0964209533333333
TotalSeconds      : 5.7852572
TotalMilliseconds : 5785.2572
```

Intel i9-9880H CPU at 2.30Ghz, 8 cores, 16 logical processors, 32.0 GB internal memory, Microsoft Windows 11.

timing a run of the script `simpson4pi1.py`

Isolating the last run:

```
from scipy.integrate import simps
from numpy import linspace, pi
from numpy.lib.scimath import sqrt
f = lambda x: sqrt(1-x**2)
r = linspace(0, 1, 10**8)
y = f(r)
I = 4*simps(y, r)
print('%.16e' % I, '%.2e' % abs(I - pi))
```

`Measure-Command {python simpson4pi1.py}`
reports 5.200 seconds.

Can we improve this?

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multiprocessing, parallelism versus concurrency

With multiprocessing we run multiple processes simultaneously.

- Each process acts as a separate program.
- The `multiprocessing` module of python enables
  - the launching of processes,
  - interprocess communication.

The multithreading in Python supports concurrency
— think of the polite dinner conversation —
not true parallelism, because of the interpreter lock.

using multiprocessing

```
from multiprocessing import Process
import os
from time import sleep

def say_hello(name, t):
    """
    Process with name says hello.
    """
    print('hello from', name)
    print('parent process :', os.getppid())
    print('process id :', os.getpid())
    print(name, 'sleeps', t, 'seconds')
    sleep(t)
    print(name, 'wakes up')
```

creating the processes

The script continues:

```
pA = Process(target=say_hello, args = ('A',2,))
pB = Process(target=say_hello, args = ('B',1,))
pA.start(); pB.start()
print('waiting for processes to wake up...')
pA.join(); pB.join()
print('processes are done')
```

running the script

The output of `python multiprocess.py` is

```
waiting for processes to wake up...
hello from A
parent process : 737
process id : 738
A sleeps 2 seconds
hello from B
parent process : 737
process id : 739
B sleeps 1 seconds
B wakes up
A wakes up
processes are done
```

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numerical integration with multiple processes

We apply domain partitioning:

$$\int_a^b f(x)dx = \sum_{i=0}^{p-1} \int_{a+i\Delta}^{a+(i+1)\Delta} f(x)dx$$

where

$$\Delta = \frac{b-a}{p}, \quad p \geq 1.$$

the script `simpson4pi2.py`

```
from multiprocessing import Process, Queue
from scipy.integrate import simps
from numpy import linspace, pi
from numpy.lib.scimath import sqrt

def call_simpson(fun, a, b, n, q):
    """
    Calls Simpson rule to integrate fun
    over [a, b] using n intervals.
    Adds the result to the queue q.
    """
    x = linspace(a, b, n)
    y = fun(x)
    I = simps(y, x)
    q.put(I)
```

the main program

```
def main():
    """
    The number of processes is given at the command line.
    """
    from sys import argv
    if len(argv) < 2:
        print('Enter the number of processes')
        print('at the command line.')
        return
    npr = int(argv[1])
```

We want to run the script as

```
python simpson4pi2.py 4
```

to time the running of the script with 4 processes.

defining processes and queues

```
crc = lambda x: sqrt(1-x**2)
nbr = 10**8
nbrsam = nbr//npr
intlen = 1.0/npr
queues = [Queue() for _ in range(npr)]
procs = []
(left, right) = (0, intlen)
for k in range(1, npr+1):
    procs.append(Process(target=call_simpson, \
        args = (crc, left, right, nbrsam, queues[k-1])))
    (left, right) = (right, right+intlen)
```

starting processes and collecting results

```
for process in procs:
    process.start()
for process in procs:
    process.join()
app = 4*sum([q.get() for q in queues])
print('%.16e' % app, '%.2e' % abs(app - pi))
```

checking for speedup

```
Measure-Command {python3 simpson4pi1.py}
```

resulted in 5.200 seconds.

Now we run

```
Measure-Command {python simpson4pi2.py 2}
Measure-Command {python simpson4pi2.py 4}
Measure-Command {python simpson4pi2.py 8}
```

to find 3.985, 3.491, and 3.518 respectively.

Computing the speedups:

1. $5.200/3.985 \approx 1.30$ with $p = 2$,
2. $5.200/3.985 \approx 1.49$ with $p = 4$,
3. $5.200/3.985 \approx 1.48$ with $p = 8$.

running times and speedups on a fast workstation

Times in seconds obtained as `time python3 simpson4pi2.py p` for `p` = 2, 4, 8, 16, and 32,
on two 22-core Intel Xeon E5-2699v4 Broadwell at 2.20GHz,
with 256GB of internal memory at 2400MHz.

For `p` = 1, `time python3 simpson4pi1.py` was used.

p	real	user	sys	speedup
1	6.586	7.766	14.135	
2	3.513	7.377	12.589	1.87
4	2.011	7.154	11.701	3.27
8	1.275	8.043	12.920	5.17
16	0.953	10.095	12.893	6.91
32	0.904	14.154	13.915	7.29

Speedups are computed as $\dfrac{\text{real time with p = 1}}{\text{real time with p tasks}}$.

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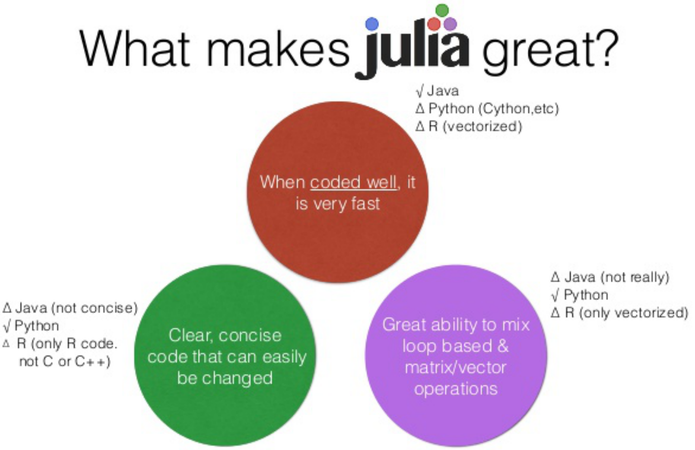
the Julia programming language

picture of Software Engineering Daily web site



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Parallel Numerical Linear Algebra

We apply multithreading in a Jupyter notebook,
in a kernel installed with the environment variable set to 16 threads.

```
julia> using IJulia
julia> installkernel("Julia (16 threads)",
       env = Dict("JULIA_NUM_THREADS"=>"16"))
```

The matrix-matrix multiplication is executed by `mul!()` of BLAS,
where BLAS stands for the Basic Linear Algebra Subroutines.

Two issues we must consider.

1. Choose the size of the matrices large enough.
2. The time should not include the compilation time.

Parallel Matrix Matrix Multiplication

The instructions in code cells of a Jupyter notebook:

```
using LinearAlgebra
n = 8000
A = rand(n, n);
B = rand(n, n);
C = rand(n, n);
BLAS.set_num_threads(2)
@time mul!(C, A, B)
```

10.722 seconds (2.87 M allocations, 5.13% compilation time)
Redo, the second time: 10.359 seconds.

```
BLAS.set_num_threads(4)
@time mul!(C, A, B)
```

6.080 seconds.

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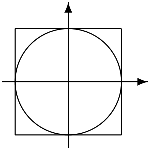
Numerical Integration

We can estimate π, via the area of the unit disk:

$$\int_0^1 \sqrt{1 - x^2} dx = \frac{\pi}{4}$$



1. Generate random uniformly distributed points with coordinates
$$(x, y) \in [0, +1] \times [0, +1].$$
2. We count a success when $x^2 + y^2 \leq 1$.

By the law of large numbers,
the average of the observed successes converges to the expected value or mean, as the number of experiments increases.

a Julia function

A dedicated random number generator is applied:

```
myrand(x::Int64) = (1103515245x + 12345) % 2^31
```

The specification of the function is below:

```
"""
    function estimatepi(n)

Runs a simple Monte Carlo method
to estimate pi with n samples.
"""
function estimatepi(n)
```

the function `estimatepi(n)`

```
function estimatepi(n)
   r = threadid()
   count = 0
   for i=1:n
       r = myrand(r)
       x = r/2^31
       r = myrand(r)
       y = r/2^31
       count += (x^2 + y^2) <= 1
   end
   return 4*count/n
end
```

running in a notebook with 16 threads

Observe the parallel for loop:

```
nt = nthreads()
estimates = zeros(nt)
import Statistics
timestart = time()

@threads for i=1:nt
    estimates[i] = estimatepi(10_000_000_000/nt)
end

estpi = Statistics.mean(estimates)
elapsed16 = time() - timestart
```

5.387

running on many threads on a fast workstation

Running version 1.4.0-DEV.364 (2019-10-22) on
two 22-core 2.2 GHz Intel Xeon E5-2699 processors
in a CentOS Linux workstation with 256 GB RAM.

p	wall clock time	elapsed time
1	1m 2.313s	62.060s
2	32.722s	32.418s
3	22.471s	22.190s
4	17.343s	17.042s
5	14.170s	13.896s
6	12.300s	11.997s
7	10.702s	10.442s

summary

Supercomputing is for everyone as most modern software provides options and tools to run on parallel machines.

- Python is a good prototyping language to define and try parallel algorithms on multicore workstations.
- Julia is a new programming language for scientific computing designed for performance.

  Ivo Balbaert, Avik Sengupta, Malcom Sherrington:
  Julia: High Performance Programming. Leverage the power of Julia to design and develop high performing programs.
  Packt Publishing, 2016.

This lecture had its focus on multiprocessing and multithreading; Python and Julia support distributed memory parallel computing.

Exercises

1. A Monte Carlo method to estimate $\pi/4$ generates random tuples (x, y), with x and y uniformly distributed in $[0, 1]$. The ratio of the number of tuples inside the unit circle over the total number of samples approximates $\pi/4$.

```
>>> from random import uniform as u
>>> X = [u(0,1) for i in xrange(1000)]
>>> Y = [u(0,1) for i in xrange(1000)]
>>> Z = zip(X,Y)
>>> F = filter(lambda t: t[0]**2 + t[1]**2 <= 1, Z)
>>> len(F)/250.0
3.1440000000000001
```

   Use the multiprocessing module to write a parallel version, letting processes take samples independently. Compute the speedup.

2. Develop a parallel Julia version for the `simpson4pi` code.