Parallel Programming in Python : a Pure-MPI code

Jiaxi Yu

Nov 06, 2020

Contents

- **the Hybrid version:**
  - structure
  - performance
  - pros and cons
- **the Pure-MPI version**
  - structure
  - performance
  - pros and cons

The Hybrid version

- **Structure:**

```
# catalogue reading using ascii.read (2e8×5 array)

# generate N uniform random array (N=30, length 2e8)
def calculation(**arg):
    # transfer N uniform array to Gaussian distributions
    # scatter a catalogue column with them
    # for each scattered array, calculate another quantity
    return mean(N quantities)

def log_like(**argv2):
    # use multiprocessing.Pool for calculation(**argv2)
    # chi_square = ((data-model)/error)**2
    return -0.5*chi_square


MC_Sampling(log_like) with mpi4py
```

The Hybrid version

- **Performance:**

```
# catalogue reading (~2min) using ascii.read (2e8×5 array)

# generate N uniform random array (~1min) (N=30, length 2e8)
def calculation (10s)(**arg):




def log like(**argv2):
    # multiprocessing.Pool(~2.5min for N=30)



MC_Sampler(log_like) with mpi4py(4.5hours for -N 16 -c 64)
```

The Hybrid version

- **Pros:**

1. easy to implement and read
2. no extra communication between processes for calculation() and MC_Sampling()

- **Cons:**

1. multiprocessing.Pool has very long communication time
2. multiprocessing.Pool only requests processes in one nodes, so N<32 and more nodes don't improve its speed

- **Expectation for MPI**

1. compute the random arrays faster
2. number of random arrays N can be larger than 32
3. faster optimisation process

The Pure-MPI version

- **Structure: Parent**

```
# initialise MPI
# catalogue reading using hdf5

def calculation(**arg):
    # Spawn N children processes
    # broadcast array size and scatter parameters to them
    # reduce the sum of all children to the root process
    return sum/N

def log_like(**argv2):
    return -0.5*((data-calculation(**argv2))/error)**2

MC_Sampler(log_like) without mpi4py
```

The Pure-MPI version

- **Structure: Children**

```
# initialise mpi4py
get parent()
receive the broadcast info


# generate a uniform random array in each parent process
# transfer this uniform array to Gaussian distributions
# scatter a catalogue column with them
# for each scattered array, calculate another quantity

reduce the sum to the root process
```

The Pure-MPI version

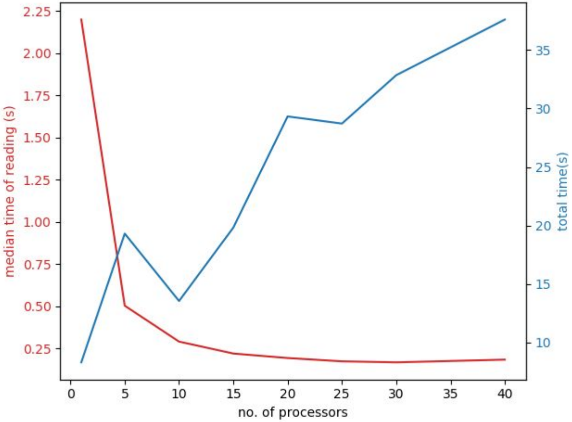
- **Performance tests:**

```
Login nodes:
Cori, 32 physical cores and 2 Threads

Computing nodes:
Haswell, 32 physical cores and 2 Threads

Memory limit:
Cori 64G, Haswell 128G

Test setting:
salloc -N 4 -n 256 -c 1 -q interactive -C Haswell
```

The Pure-MPI version

- **Performance tests:**

```
# reading catalogue using hdf5:
```




```
data will gather in the
end of reading
```

↓

```
long communication time
& no enough memory
```

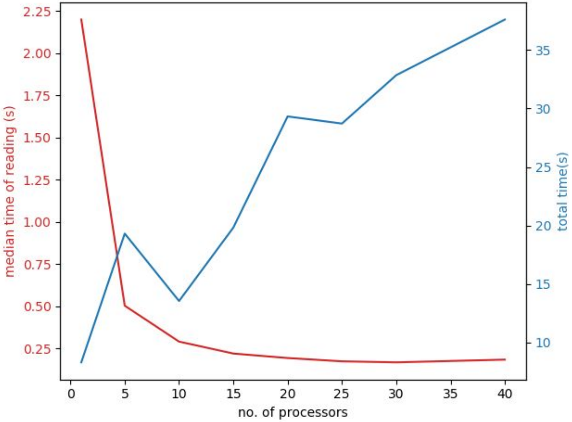
↓

```
 no need to parallelise
(still much better than
2-min ascii reading )
```

The Pure-MPI version

- **Performance tests:**

reading catalogue using hdf5:



data will gather in the end of reading

↓

long communication time & no enough memory

↓

no need to parallelise

* mpiexec -n 64: 74s
* mpiexec -n 128: >370s

The Pure-MPI version

- **Performance tests:**

```
# parent-child structure tests
x = np.linspace(0.,101.,int(8e7))
maxproc = #
def log_like(argv):
    model  = par[0]*x+par[1]
    comm   = MPI.COMM_SELF.Spawn (sys.executable,
                         args=[' child.py'],maxprocs=maxproc)
    lenx   = np.array(len(x),'i')
    sigma  = np.array(1.,'d')
    comm.Bcast ([lenx, MPI.INT], root=MPI.ROOT)
    comm.Bcast ([sigma, MPI.DOUBLE], root=MPI.ROOT)
    noise  = np.zeros(lenx,'d')
    comm.Reduce (None,[noise,MPI.DOUBLE],op=MPI.SUM, root=MPI.ROOT)
    y_mean = 2*x+3+noise/maxproc
    comm.Disconnect()
    return -0.5*((y_mean-model)**2/error**2).sum()

print(log_like([a,b]))
```

The Pure-MPI version

- **Performance tests:**

```
# parent-child structure tests
'child.py'

# initialise mpi4py
lenx    = np.array(0.,'i')
sigma   = np.array(0.,'d')
comm.Bcast([lenx, MPI.INT], root=0)
comm.Bcast([sigma, MPI.DOUBLE], root=0)

# make sure the Gaussian random is stable
uniform = np.random.RandomState(seed=rank+1).rand(lenx)
half    = int(lenx/2)
noise    =
append(sigma*sqrt(-2*log(uniform[:half]))*cos(2*pi*uniform[half:])
,\
sigma*sqrt(-2*log(uniform[:half]))*sin(2*pi*uniform[half:]))

comm.Reduce([noise,MPI.DOUBLE],None,op=MPI.SUM, root=0)
comm.Disconnect()
```

The Pure-MPI version

- **Performance tests:**

```
# parent-child structure tests

x = np.linspace(0.,101.,int(8e7)) # close to the upper memory
limit

maxproc (number of children processes)
> mpiexec -n Ntask python parent.py (A parent processes)


# baseline 1
replace children with multiprocessing.Pool with 30 processes

# baseline 2
Nnodes = 2, maxproc = 30, ntasks = A = 2
```

The Pure-MPI version

- **Performance tests:**

```
# parent-child structure tests
```

	Nnode	ntask	maxproc	time(s)
base1	2	2	30	145.0
base2	2	2	30	37.05
MPI	4	2	30	44.24
MPI	4	2	60	46.44

The Pure-MPI version

- **Performance tests:**

```
#  likelihood combined with the Monte-Carlo Sampler
```

(Problematic!)

1. **Pymultinest: cannot work at all even though its own mpi4py is disabled**

2. **emcee: a sequential code. But it stops after 17% points are sampled (no error reports).**

The Pure-MPI version

- **Pros:**
  1. maxproc can be larger than 30
  2. random array has been generated 3 times faster than the hybrid version
- **Cons:**
  1. difficult to adjust to the external library
  2. easily out of memory given the large data set, so data-preprocessing needed
- **Code&results:**

  https://github.com/Jiaxi-Yu/parallel_programming_project.git

Thanks!

The Hybrid version:C

Self	ELF Object
57.82	libm-2.17.so
23.12	libc-2.17.so
18.84	MTSHAM
0.21	libpthread-2.17.so
0.00	ld-2.17.so
0.00	libnuma.so.1.0.0
0.00	libgfortran.so.3.0.0

Incl.	Self	Called	Function	Location
100.00	0.00	1	0x0000000000402c27	MTSHAM
100.00	0.00	1	main	MTSHAM
74.84	0.00	1	save_best	MTSHAM
74.84	0.00	1	best_fit	MTSHAM
74.53	3.93	102	apply_sham	MTSHAM
70.56	9.93	17 833 783 221	mt19937_get_gauss	MTSHAM
25.16	0.00	1	read_cata	MTSHAM
25.16	0.87	1	read_ascii_data	MTSHAM
2.81	2.81	8 916 891 611	mt19937_get	MTSHAM
0.50	0.50	881 673 180	ast_set_var	MTSHAM
0.50	0.39	881 673 180	ast_eval	MTSHAM
0.30	0.00	101	comp_2pcf_auto	MTSHAM
0.21	0.00	101	kdtree_count_auto_pairs	MTSHAM
0.21	0.00	101	kdtree_dual_auto_intbi...	MTSHAM
0.21	0.21	28 220 463	kdtree_dual_auto_intbi...	MTSHAM
0.11	0.11	881 673 180	ast_eval_double.part.3	MTSHAM
0.09	0.01	101	kdtree_build	MTSHAM
0.08	0.08	1 654 582	kdtree_build'2	MTSHAM
0.01	0.01	93 738 432	compare_mass	MTSHAM

C-profiling costs 6 hours
& gprof didn't work
& data all in ascii format

The Pure-MPI version

- **Structure:**

failed due to unnoticed deadlock

```
# generate N uniform random array
def calculation(**arg):
    # transfer N uniform array to Gaussian distributions
    # scatter a catalogue column with them
    # for each scattered array, calculate another quantity
    return mean(N quantities)

def log_like(**argv2):
    # use MPI.Pool for calculation(**argv2)
    # chi_square = ((data-model)/error)**2
    return -0.5*chi_square


a serial MC_Sampler(log_like)
```