Maximizing parallelizaton of BLAST: Output Formatting Section (OFS)

Albert Golembiowski, Ph.D.

Intel® Corporation

Objectives

- get the last serial section (OFS) in runtime blast(n/p) to parallelize
- Improve throughput performance of the heterogeneous load sharing Xeon® – XeonPhi ® model, for multiple concatenated queries and multiple db volumes (model #4).

Benchmark configurations

- Intel ® Xeon ® Two 12-Core E5-2697 v2, 2.7GHz (IVT)
- Intel ® Xeon Phi® 7120A (KNC)
- BLAST version 2.2.29, code base retrieved from NCBI website.
- NCBI provided 100 BLASTn benchmarks.
- Multiple query/multiple db command line options are:

```
> blastn_mic –task blastn –db ‘db/refseq_rna.00 db/refseq_rna.01
db/refseq_rna.02’ –query queries/blastn/NM_5_concat –num_threads 180
```

Query model and Xeon® – XeonPhi ® experiment

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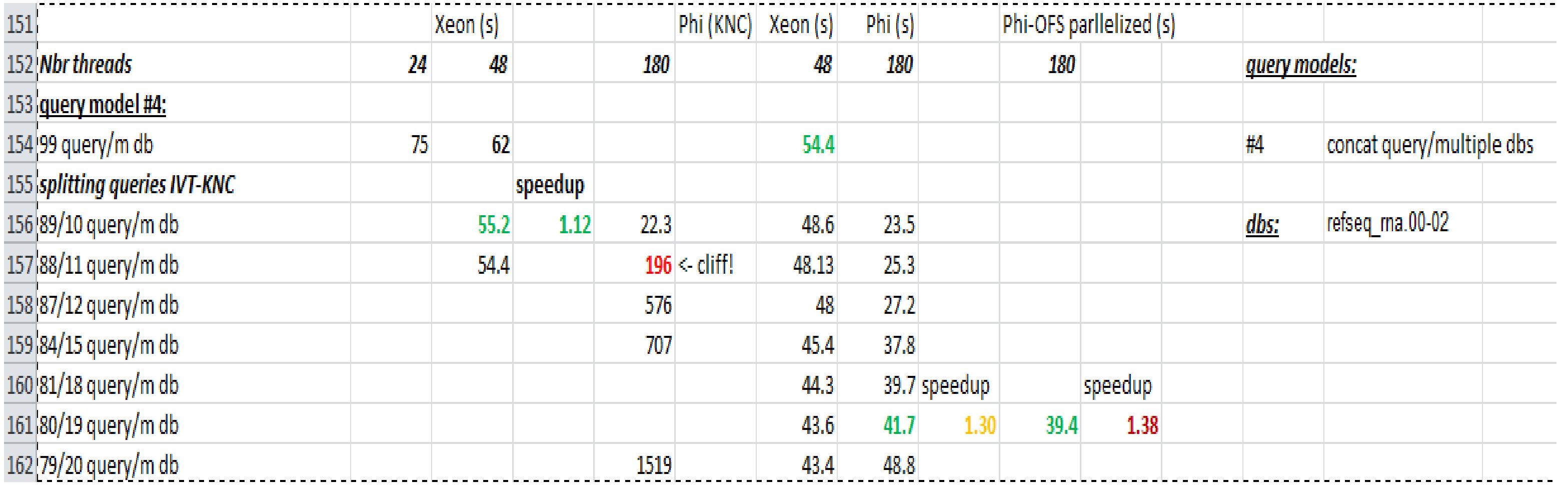
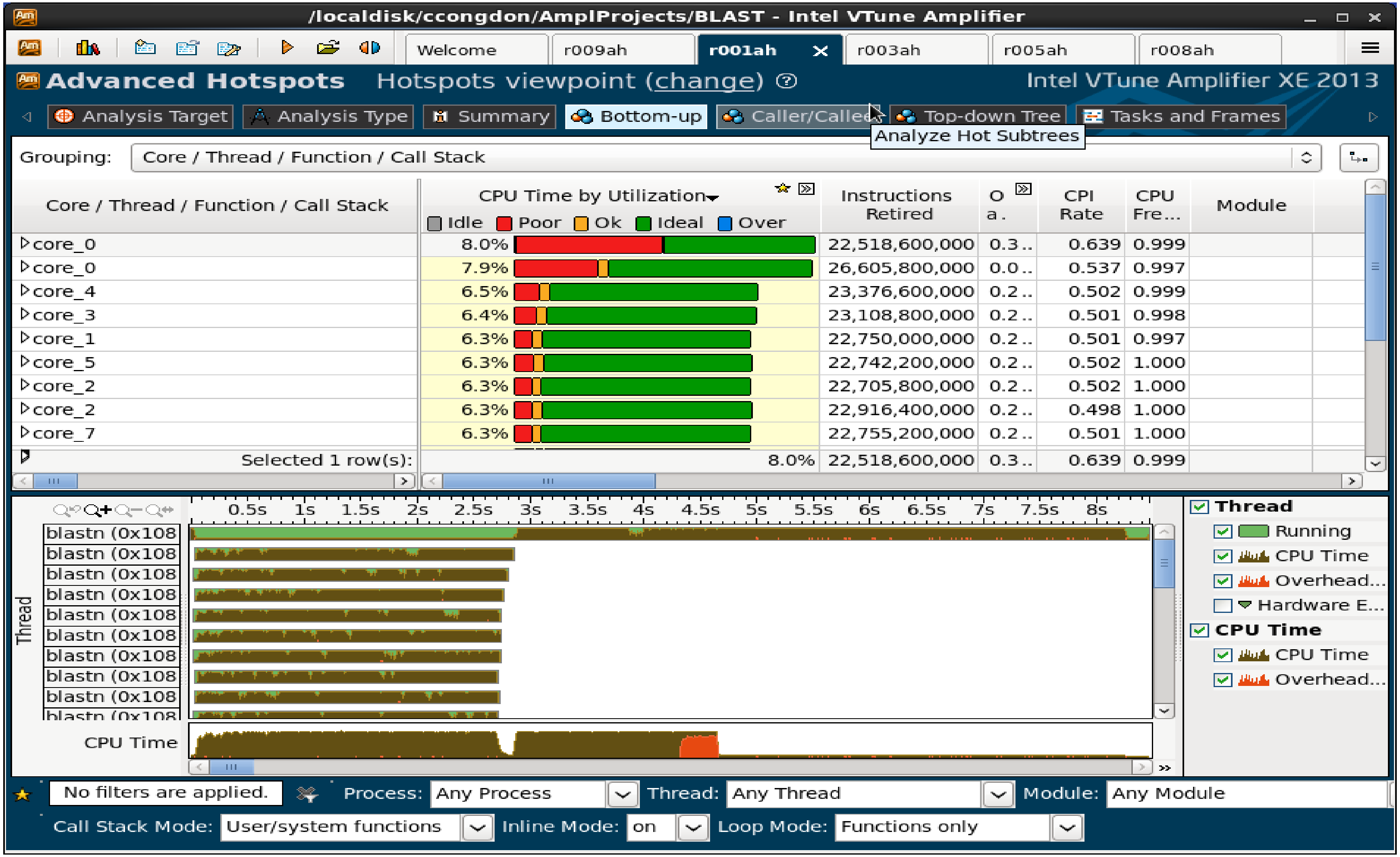


151			Xeon (s)			Phi (KNC)	Xeon (s)	Phi (s)		Phi-OFS parllelized (s)				
152	***Nbr threads***	***24***	***48***		***180***		***48***	***180***		***180***			***query models:***	
153	**query model #4:**													
154	99 query/m db	75	62				54.4						#4	concat query/multiple dbs
155	***splitting queries IVT-KNC***			**speedup**										
156	89/10 query/m db		55.2	1.12	22.3		48.6	23.5					***dbs:***	refseq_rna.00-02
157	88/11 query/m db		54.4		196	<- cliff!	48.13	25.3						
158	87/12 query/m db				576		48	27.2						
159	84/15 query/m db				707		45.4	37.8						
160	81/18 query/m db						44.3	39.7	speedup		speedup			
161	80/19 query/m db						43.6	41.7	1.30	39.4	1.38			
162	79/20 query/m db				1519		43.4	48.8						

The 80 concatenated queries on Xeon (IVT) and 19 queries on KNC, in heterogeneous load sharing model (#4) run concurrently in 41.7s and 39.4s respectively, as compared to all 99 concatenated queries on Xeon 54.4s. Here the speedup is 1.3x and ~1.4x for OFS parallelized

BLASTN: single query/single db (model #1)



/localdisk/ccongdon/AmplProjects/BLAST - Intel VTune Amplifier

Welcome | r009ah | r001ah | r003ah | r005ah | r008ah

Advanced Hotspots Hotspots viewpoint (change) Intel VTune Amplifier XE 2013

Analysis Target | Analysis Type | Summary | Bottom-up | Caller/Callee | Top-down Tree | Tasks and Frames

Analyze Hot Subtrees

Grouping: Core / Thread / Function / Call Stack

Core / Thread / Function / Call Stack	CPU Time by Utilization ■ Idle 🟥 Poor 🟧 Ok 🟩 Ideal 🟦 Over	Instructions Retired	O a.	CPI Rate	CPU Fre...	Module
▷core_0	8.0%	22,518,600,000	0.3..	0.639	0.999	
▷core_0	7.9%	26,605,800,000	0.0..	0.537	0.997	
▷core_4	6.5%	23,376,600,000	0.2..	0.502	0.999	
▷core_3	6.4%	23,108,800,000	0.2..	0.501	0.998	
▷core_1	6.3%	22,750,000,000	0.2..	0.501	0.997	
▷core_5	6.3%	22,742,200,000	0.2..	0.502	1.000	
▷core_2	6.3%	22,705,800,000	0.2..	0.502	1.000	
▷core_2	6.3%	22,916,400,000	0.2..	0.498	1.000	
▷core_7	6.3%	22,755,200,000	0.2..	0.501	1.000	
Selected 1 row(s):	8.0%	22,518,600,000	0.3..	0.639	0.999	

☑ Thread
☑ Running
☑ CPU Time
☑ Overhead...
□ Hardware E...
☑ CPU Time
☑ CPU Time
☑ Overhead...

No filters are applied. Process: Any Process Thread: Any Thread Module: Any Module

Call Stack Mode: User/system functions Inline Mode: on Loop Mode: Functions only

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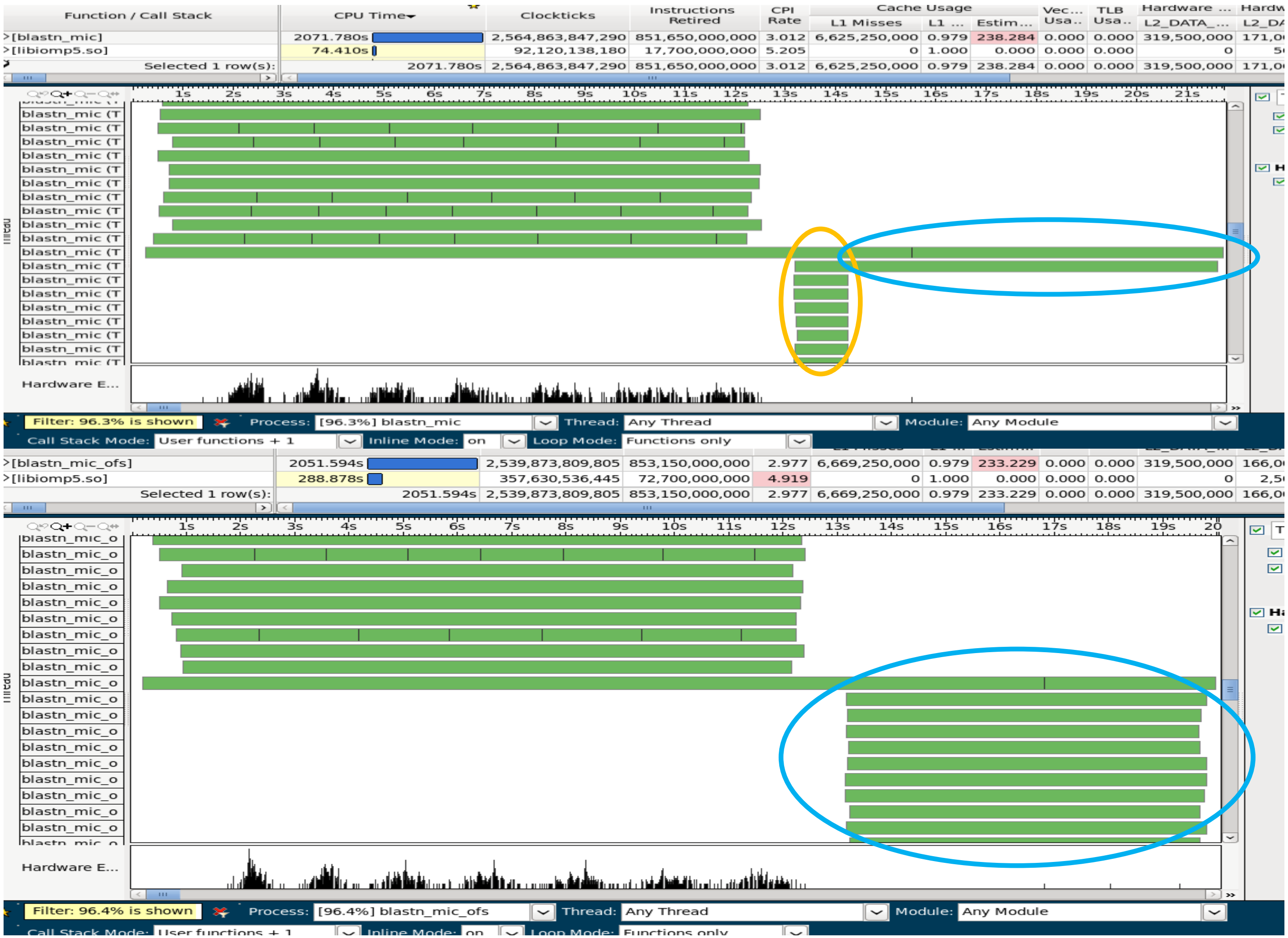
Clearly are visible the 3 sections on "CPU Time". (1) preliminary search (pthread parallelized), (2) traceback search (omp parallelized), and (3) output formatting (serial)

Parallelizing OFS: strategy and implementation

- Identify top level loop and the one with most iterations (key loop)
- Clone/initialize the `display’ (CDisplaySeqalign::) object one clone per thread.
- Break up key loop into NT iteration chunks (equalize workload)
- Identify key loop global object changing state per iteration and make NT clones.
- Spin up clones to a correct initial state.
- Give each iteration chunk to one thread
- Eliminate thread data contentions (mutexes) for maximum speed
- Use LTS std::ostringstream object (STR_STREAM) per thread for output
- Reduce NT STR_STREAM objects into the original NcbiOstrStream output

BLASTN: 5 concat queries on KNC running 180T (model #4)



Function / Call Stack	CPU Time	Clockticks	Instructions Retired	CPI Rate	Cache Usage L1 Misses	L1 ...	Estim...	Vec... Usa..	TLB Usa..	Hardware ... L2_DATA_...	Hardw L2_DA
>[blastn_mic]	2071.780s	2,564,863,847,290	851,650,000,000	3.012	6,625,250,000	0.979	238.284	0.000	0.000	319,500,000	171,0
>[libiomp5.so]	74.410s	92,120,138,180	17,700,000,000	5.205	0	1.000	0.000	0.000	0.000	0	5
Selected 1 row(s):	2071.780s	2,564,863,847,290	851,650,000,000	3.012	6,625,250,000	0.979	238.284	0.000	0.000	319,500,000	171,0

Filter: 96.3% is shown Process: [96.3%] blastn_mic Thread: Any Thread Module: Any Module

Call Stack Mode: User functions + 1 Inline Mode: on Loop Mode: Functions only

>[blastn_mic_ofs]	2051.594s	2,539,873,809,805	853,150,000,000	2.977	6,669,250,000	0.979	233.229	0.000	0.000	319,500,000	166,0
>[libiomp5.so]	288.878s	357,630,536,445	72,700,000,000	4.919	0	1.000	0.000	0.000	0.000	0	2,5
Selected 1 row(s):	2051.594s	2,539,873,809,805	853,150,000,000	2.977	6,669,250,000	0.979	233.229	0.000	0.000	319,500,000	166,0

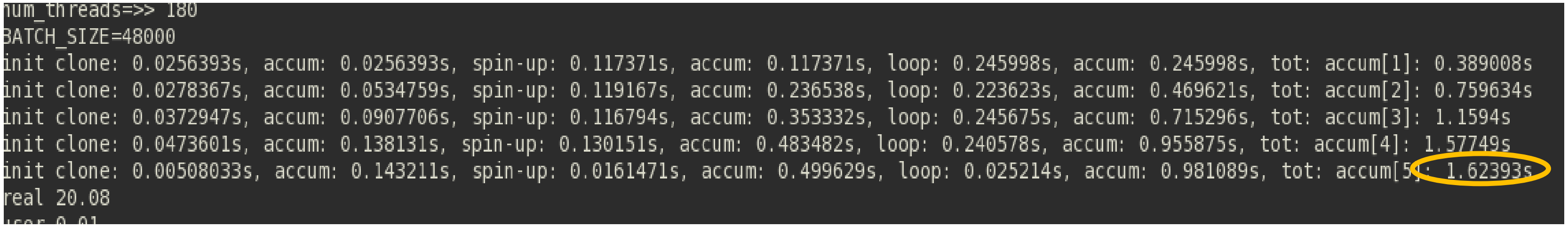
Filter: 96.4% is shown Process: [96.4%] blastn_mic_ofs Thread: Any Thread Module: Any Module

Call Stack Mode: User functions + 1 Inline Mode: on Loop Mode: Functions only

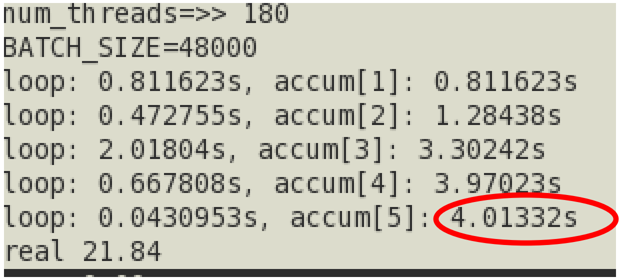
1s 2s 3s 4s 5s 6s 7s 8s 9s 10s 11s 12s 13s 14s 15s 16s 17s 18s 19s 20s 21s
blastn_mic (T
Hardware E...
1s 2s 3s 4s 5s 6s 7s 8s 9s 10s 11s 12s 13s 14s 15s 16s 17s 18s 19s 20
blastn_mic_o
Hardware E...

(1) GAT parallelized, (2) output formatting section (OFS) parallelized. i/o inhibited by writing output into /dev/null.

BLASTN: OFS parallelization re-arch



```
num_threads=>> 180
BATCH_SIZE=48000
init clone: 0.0256393s, accum: 0.0256393s, spin-up: 0.117371s, accum: 0.117371s, loop: 0.245998s, accum: 0.245998s, tot: accum[1]: 0.389008s
init clone: 0.0278367s, accum: 0.0534759s, spin-up: 0.119167s, accum: 0.236538s, loop: 0.223623s, accum: 0.469621s, tot: accum[2]: 0.759634s
init clone: 0.0372947s, accum: 0.0907706s, spin-up: 0.116794s, accum: 0.353332s, loop: 0.245675s, accum: 0.715296s, tot: accum[3]: 1.1594s
init clone: 0.0473601s, accum: 0.138131s, spin-up: 0.130151s, accum: 0.483482s, loop: 0.240578s, accum: 0.955875s, tot: accum[4]: 1.57749s
init clone: 0.00508033s, accum: 0.143211s, spin-up: 0.0161471s, accum: 0.499629s, loop: 0.025214s, accum: 0.981089s, tot: accum[5]: 1.62393s
real 20.08
user 0.01
```

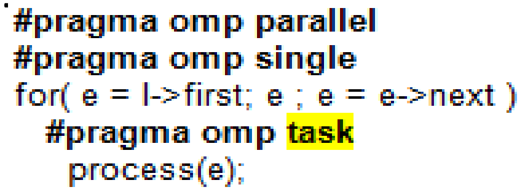


```
num_threads=>> 180
BATCH_SIZE=48000
loop: 0.811623s, accum[1]: 0.811623s
loop: 0.472755s, accum[2]: 1.28438s
loop: 2.01804s, accum[3]: 3.30242s
loop: 0.667808s, accum[4]: 3.97023s
loop: 0.0430953s, accum[5]: 4.01332s
real 21.84
```

(a) parallelized OFS: breakdown of time spent in key loop vs overhead introduced , (b) serial OFS: original loop timing

Things to try

- Resolve icc issue building blastp (workaround identified)
- Reduce OFS parallelization overhead
  - Current implementation of cloning maybe too heavy?
  - try omp



```
#pragma omp parallel
#pragma omp single
for( e = l->first; e ; e = e->next )
   #pragma omp task
     process(e);
```

- Parallelize GAT for blastp.

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