

1000 Downloads of Genetically Improved DNA Analysis Software

CREST Open Workshop on Genetic Improvement 25-26 January 2016

[W. B. Langdon](#)

Computer Science, University College London



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Genetic Improvement



CEC 2016, Vancouver, 25-29 July 2016
[Special Session](#) on Genetic Improvement

Based on GECCO 2015 [p1063-1070](#)

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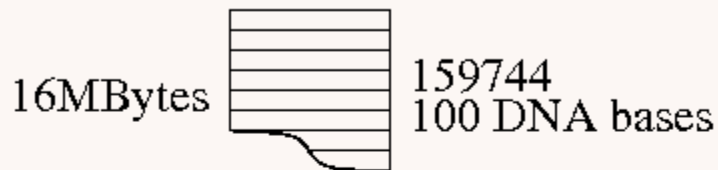
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What is BarraCUDA ?

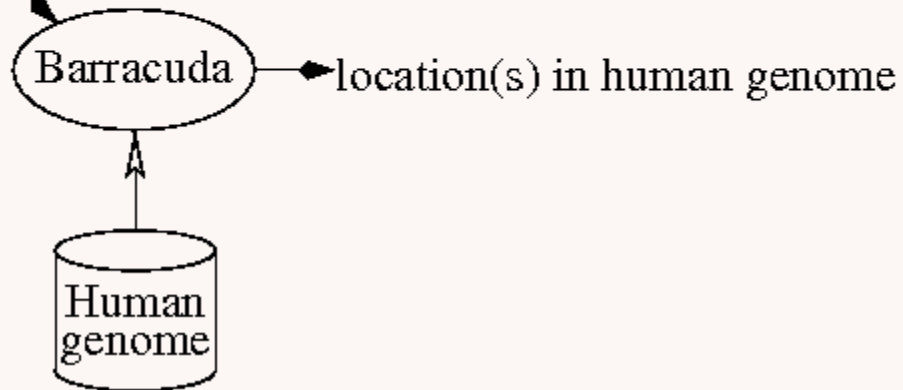
DNA analysis program

- 8000 lines C code, SourceForge.
- Rewrite of BWA for nVidia CUDA

tens of millions of short DNA sequences

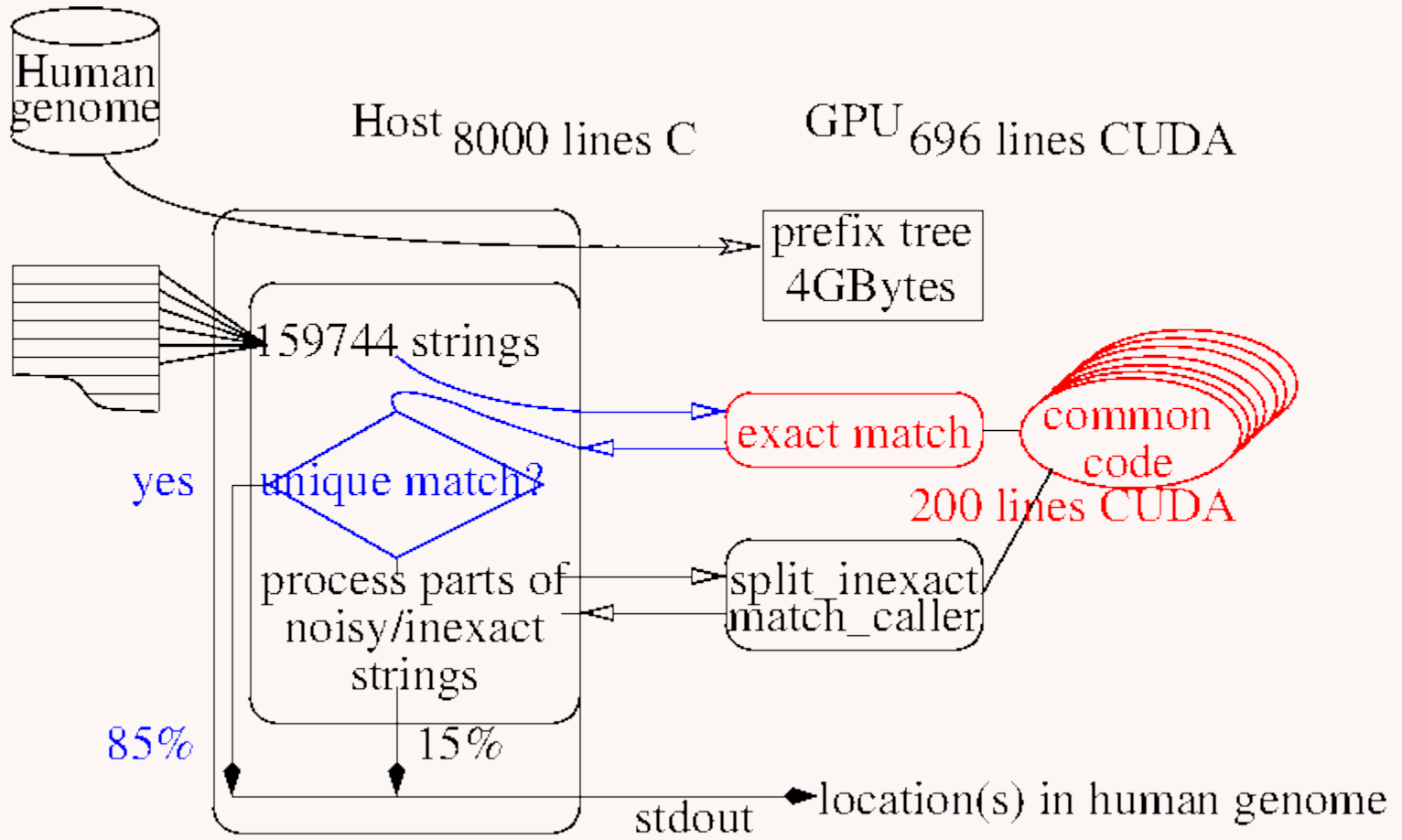


Speed comes from processing 159,744 strings in parallel on GPU



BarraCUDA 0.7.107b

Manual host changes to call exact_match kernel
GI parameter and code changes on GPU



Why 1000 Genomes Project ?

- Data typical of modern large scale DNA mapping projects.
- Flagship bioinformatics project
 - Project mapped all human mutations.
- 604 billion short human DNA sequences.
- Download raw data via FTP

\$120million [180Terra Bytes](#)

Preparing for Evolution

- Re-enable **exact matches** code
- **Support 15 options**(conditional compilation)
- Genetic programming fitness testing framework
 - Generate and compile 1000 unique mutants
 - Whole population in one source file
 - Remove mutants who fail to compile and then re-run compiler to compile the others
 - Run and measure speed of 1000 kernels
 - Reset GPU following run time errors
 - For each kernel check 159444 answers

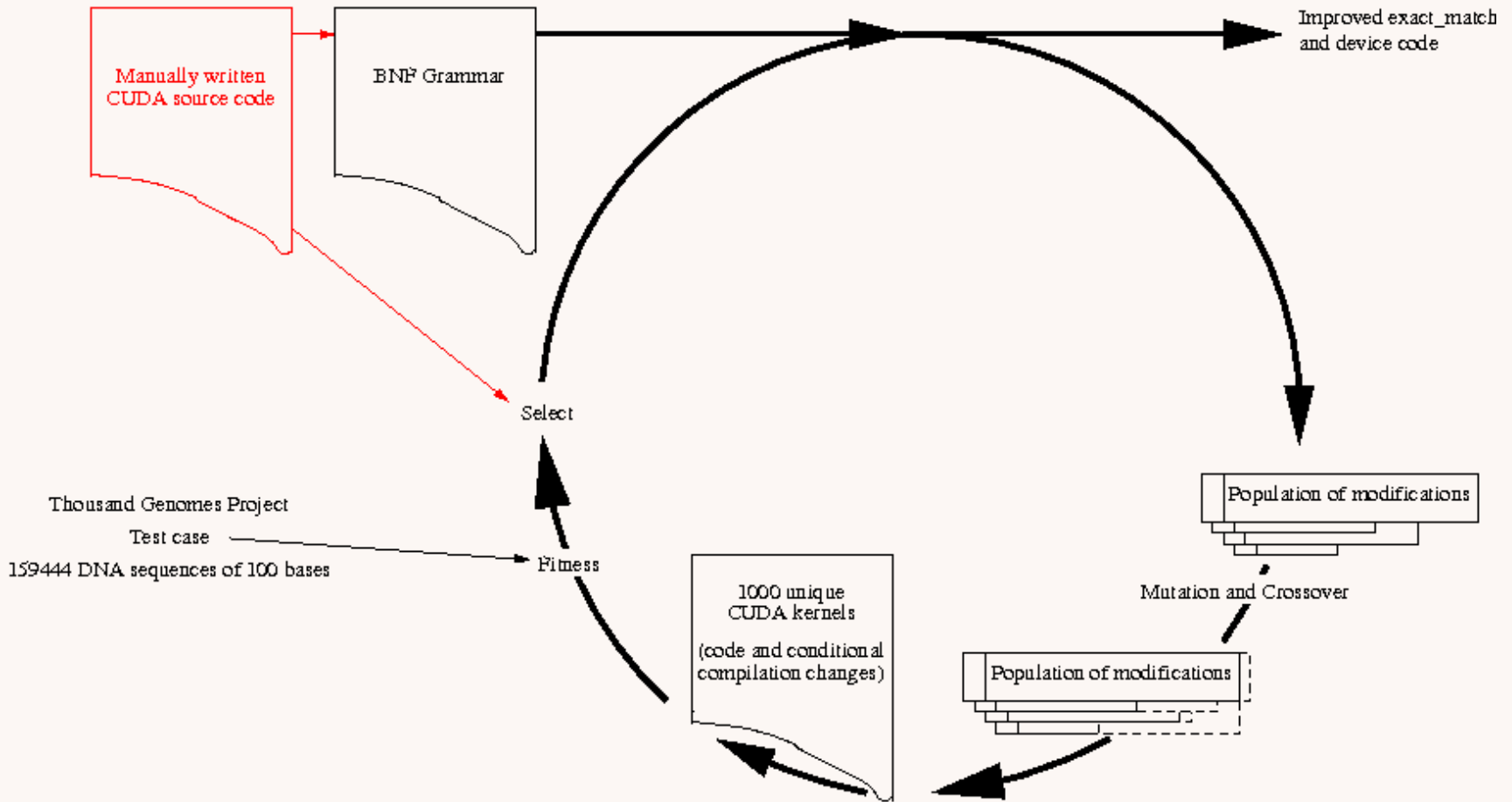
Fixed Parameters

Parameter		default	Lines of code affected
BLOCK_W	int	64	all
cache_threads	"" int	""	44
kl_par	binary	off	19
occ_par	binary	off	76
many_blocks	binary	off	2
direct_sequence	binary	on	63
direct_index	binary	on	6
sequence_global	binary	on	16
sequence_shift81	binary	on	30
sequence_stride	binary	on	14
mycache4	binary	on	12
mycache2	binary	off	11
direct_global_bwt	binary	off	2
cache_global_bwt	binary	on	65
scache_global_bwt	binary	off	35

Evolving BarraCUDA kernel

- Convert manual CUDA code into grammar
- Grammar used to control code modification
- GP manipulates patches and fixed params
 - Small movement/deletion of existing code
 - New program source is syntactically correct
 - Automatic scoping rules ensure almost all mutants compile
 - Force loop termination
- Genetic Programming continues despite compilation and runtime errors

Evolving BarraCUDA



50 generations in 11 hours

W. B. Langdon, UCL

BNF Grammar

Configuration
parameter

```

if (*lastpos!=pos_shifted)
{
#ifdef sequence_global
    *data = tmp = tex1Dfetch(sequences_array, pos_shifted);
#else
    *data = tmp = Global_sequences(global_sequences,pos_shifted);
#endif /*sequence_global*/
    *lastpos=pos_shifted;
}

```

CUDA lines 119-127

```

<119> ::= " if" <IF_119> " \n"
<IF_119> ::= " (*lastpos!=pos_shifted) "
<120> ::= "{\n"
<121> ::= "#ifdef sequence_global\n"
<122> ::= "" <_122> "\n"
<_122> ::= "*data = tmp = tex1Dfetch(sequences_array, pos_shifted);"
<123> ::= "#else\n"
<124> ::= "" <_124> "\n"
<_124> ::= "*data = tmp = Global_sequences(global_sequences,pos_shifted);"
<125> ::= "#endif\n"
<126> ::= "" <_126> "\n"
<_126> ::= "*lastpos=pos_shifted;"
<127> ::= "}\n"

```

Fragment of Grammar (Total 773 rules)

9 Types of grammar rule

- Type indicated by rule name
- Replace rule only by another of same type
- 650 fixed, 115 variable.
- 43 statement (e.g. assignment, **Not** declaration)
- 24 IF
 - `<_392> ::= " if" <IF_392> " {\n"`
 - `<IF_392> ::= " (par==0)"`
- Seven for loops (for1, for2, for3)
 - `<_630> ::= <okdeclaration_> <pragma_630>`
`"for(" <for1_630> ";" "OK()&&" <for2_630> ";" <for3_630> ") \n"`
- 2 ELSE
- 29 CUDA specials

Representation



- 15 fixed parameters; variable length list of grammar patches.
 - no size limit, so search space is infinite
- Uniform crossover and tree like 2pt crossover.
- Mutation flips one bit/int or adds one randomly chosen grammar change
- 3 possible grammar changes:
 - Delete line of source code (or replace by "", 0)
 - Replace with line of GPU code (same type)
 - Insert a copy of another line of kernel code

Example Mutating Grammar

```
<_947> ::= "*k0 = k;"  
<_929> ::= "((int*)l0)[1] =  
__shfl(((int*)&l)[1], threads_per_sequence/2, threads_per_sequence);  
"
```

2 lines from grammar

`<_947>+<_929>`

Fragment of list of mutations

Says insert copy of line 929 before line 947

Copy of line 929



New code

```
((int*)l0)[1] =  
__shfl(((int*)&l)[1], threads_per_sequence/2, threads_per_sequence);  
*k0 = k;
```

Line 947

Recap

- Representation
 - 15 fixed genes (mix of Boolean and integer)
 - List of changes (delete, replace, insert).
New rule must be of same type.
- Mutation
 - 1 bit flip or small/large change to int
- append one random change to `codeCrossover`
 - Uniform GA crossover
 - GP tree like 2pt crossover
- Evolve for 50 generations

Best K20 GPU Patch in gen 50

Parameter		new
scache_global_bwt	off	on
cache_threads	off	2
BLOCK_W	64	128

Store bwt cache in registers
 Use 2 threads to load bwt cache
 Double number of threads

line	Original Code	New Code
635		#pragma unroll
578	if(k == bwt_cuda.seq_len)	if(0)
947	*k0 = k;	((int*)l0)[1] = __shfl(((int*)&l)[1], threads_per_sequence/2, threads_per_sequence); *k0 = k;
126	*lastpos=pos_shifted;	

Line 578 if was never true

l0 is overwritten later regardless

Change 126 disables small sequence cache 3% faster

Results

- Ten randomly chosen 100 base pair datasets from 1000 genomes project:
 - K20 1 840 000 DNA sequences/second (original 15000)
 - K40 2 330 000 DNA sequences/second (original 16 000)
- 100% identical
- manually incorporated into sourceForge
- 1068 downloads (10 months)

GI: To Do List

- Systems
 - [GenProg](#)
- Wikipedia
- ~~Bibliography?~~
- GI [workshop](#) (Denver), [GI@CEC](#) (Vancouver)
- Other resources: www, email, discussion???
- How to do Genetic Improvement
 - Documentation
 - Tutorials
 - Little examples. Real benchmarks



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Conclusions

- Genetic programming
 - Compile into one executable
 - Scoping rules
 - Run compiler until all remaining code compiles
 - Fitness test representative data v. existing code
- On real typical data raw speed up > 100 times
- Impact diluted by rest of code
- On real data speed up can be >3 times (arXiv.org)
- Incorporated into real system
 - 1st use of genetic improvement

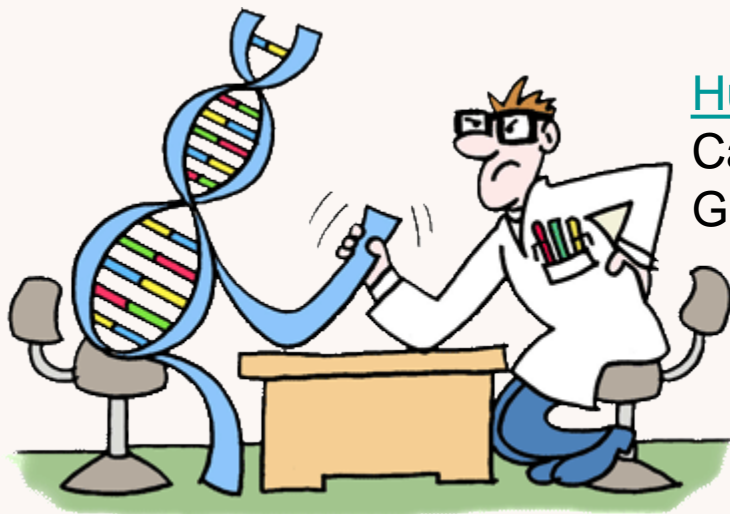




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Humies: Human-Competitive
Cash prizes
GECCO-2016

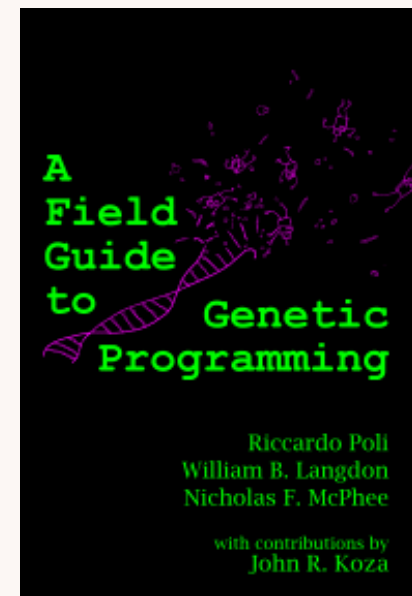
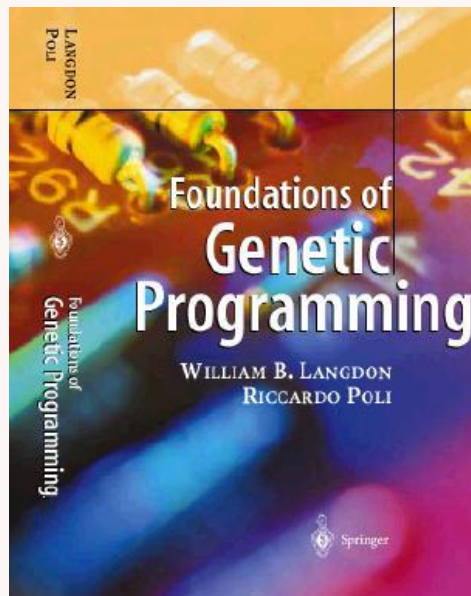
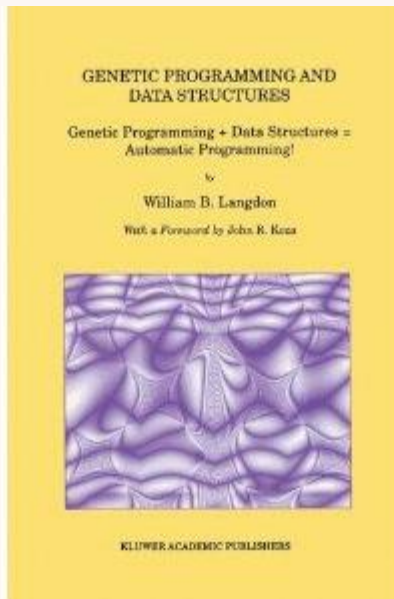
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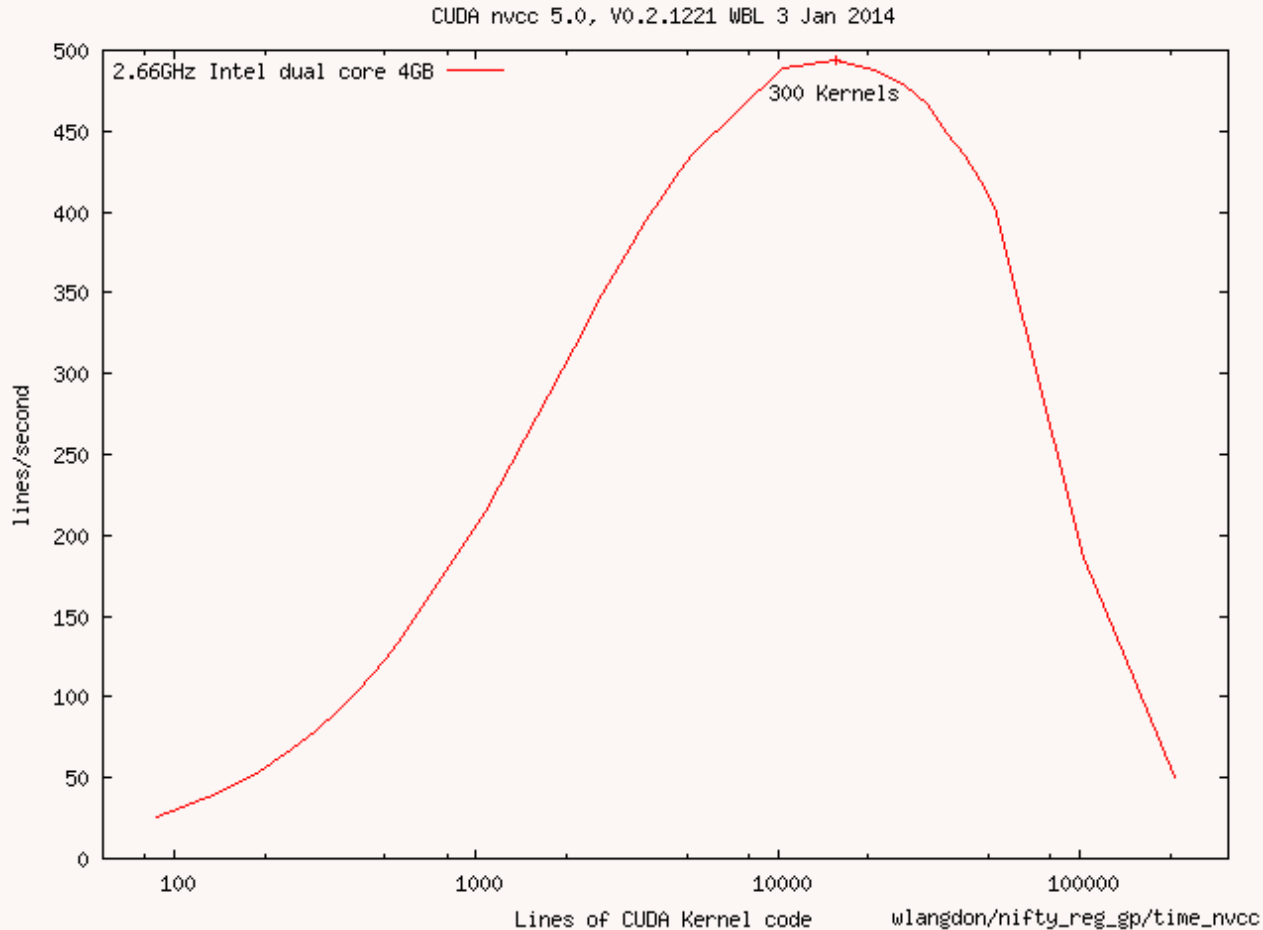
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Conclusions

- Genetic programming can automatically re-engineer source code. E.g.
 - hash algorithm
 - Random numbers which take less power, etc.
 - mini-SAT ([Humie](#) award)
- fix bugs ($>10^6$ lines of code, 16 programs)
- create new code in a new environment (graphics card) for existing program, gzip [WCCI '10](#)
- new code to extend application (GGGP) [SSBSE'14](#)
- speed up GPU image processing [EuroGP'14](#)
[GECCO'14](#)
- speed up 50000 lines of code [IEEE TEC](#)
10000 speed up [GI-2015](#)

Compile Whole Population



Note Log x scale

Compiling many kernels together is about 20 times faster than running the compiler once for each.

CUDA specials and configuration parameters

- BNF special types for CUDA
 - `optrestrict` apply `__restrict__` to all pointer arguments
 - `launchbounds` applies on starting CUDA kernel
 - `#pragma unroll`
- 15 Parameters
 - Macro `#define` holds value of parameter
 - Macro used in code, e.g. via conditional compilation
 - Cleared with `#undef` before next mutant is compiled

Example2 Mutating Grammar

```
<_Kkernel_bnf.cu_126> ::= "*lastpos=pos_shifted;"
```

1 line from grammar

<_126>

Fragment of list of mutations
Says delete line 126

Testing exact_match kernel variants

- Apply 1000 GP patches (plus original)
- Compile specifically for GPU in use.
- Run on 159744 randomly chosen 100 base pair DNA sequences (fixed sequence).
- Calculate time taken and check answers.
- Only those returning correct answers quicker than manual code can breed.
- Choose fastest 500 to be parents.
- Mutate, crossover: 2 children per parent.
- Repeat 50 generations.

Run time errors

- Automated scoping rules ensure during evolution 96.5% compile. (Each BNF rule annotated with line numbers where it can be copied to.)
 - Mutants which fail to compile are removed and then compiler is re-run
- Almost all kernels run and terminate
 - Long running loops are aborted by OK() macro
 - Index out of array bounds are ignored
 - Modern GPUs more resilient to bad code
 - Hardware reported exceptions cause host to reset GPU before testing next kernel.
- Errors implicitly lead to poor fitness: long run times or incorrect answers.

GP Evolution Parameters

- Pop 1000, 50 generations
- 50% crossover:
 - 25% uniform crossover on fixed parameters
 - 25% tree like two point crossover on variable length list of code patches
- 50% mutation
 - 25% change one fixed parameter (bit flip, BLOCK_W another legal value, either adjacent or random).
 - 25% add a random patch to variable list.
- Truncation selection
- \approx 11 hours

GP Automatic Coding

- Use existing code as test “Oracle”.
(Program is its own functional specification)

Scope

- Line can be copied where all its vars are in scope
- `<IF_Kkernel_bnf.cu_119>` line 109 to 168
`if (*lastpos!=pos_shifted)`
- Line 99 `unsigned int * lastpos,`
- Line 109 `unsigned const int pos_shifted = ..`
- Line 168 `}` end of function `read_char()`

Comparisons

- Barracuda before and after GI
- BWA (12 cores)
- Bowtie2
- nvBowtie2

GPUs

GPU	Total cores	clock	Bandwidth Giga Bytes/sec
GeForce GT 730	96	1.40 GHz	23
Tesla K20	2496	0.71 GHz	140
Tesla K40	2880	0.88 GHz	180
Tesla K80	2496	0.82 GHz	138

Tesla K80 is dual GPU. Figures given for one half.

DNA sequences per second

Prog	Length	12 core 2.60GHz CPU	GT 730	2 K20	K80	GCAT accuracy
BWA	36bp	1900				
	100bp	4500				98.91%
Old Barracuda	36bp		3270	5300	6500	
	100bp		1860	8700	11700	97.49%
New Barracuda	36bp		7600	12900	19900	
	100bp		2100	8800	1280	98.43%

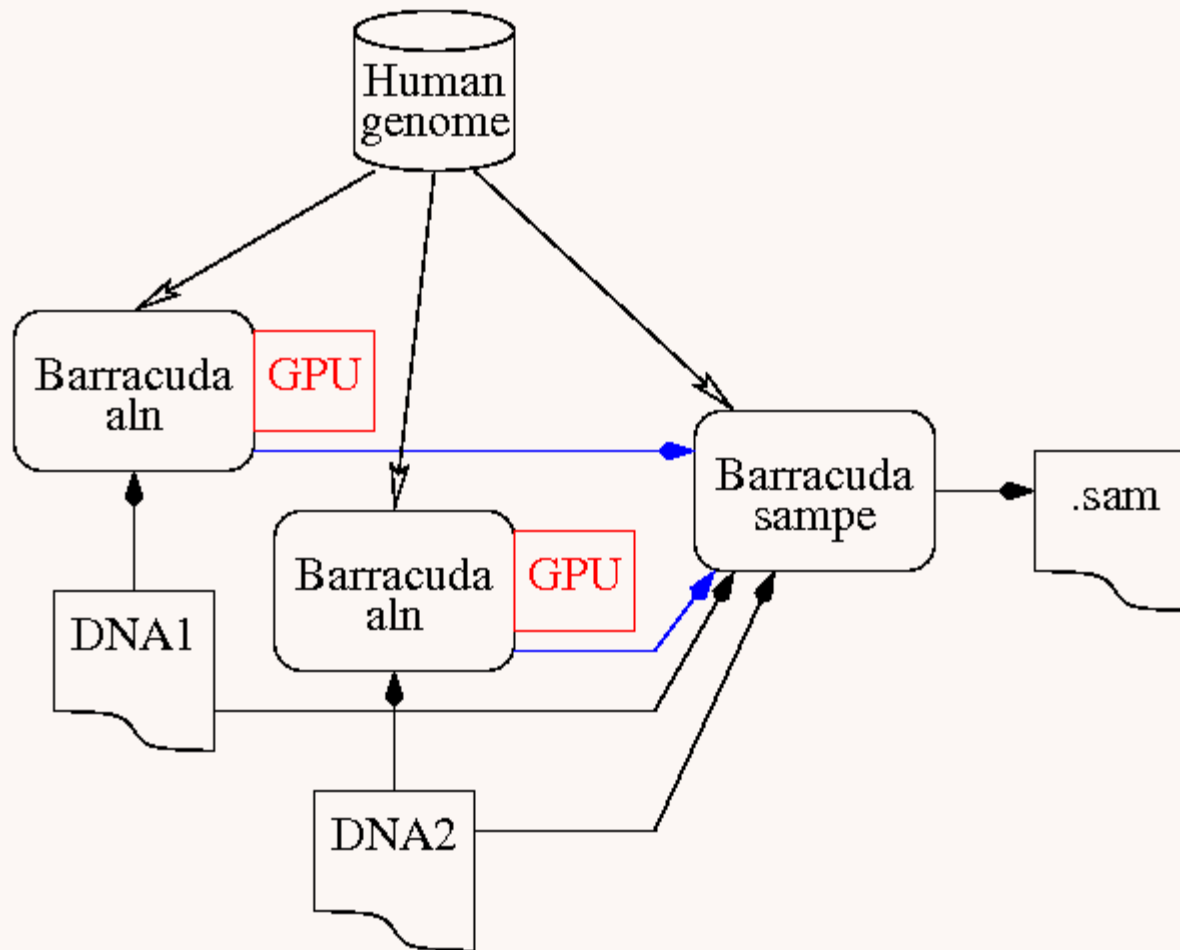
- Twin GPUs work on each of paired ends
- GT730 estimated as if two in use

DNA sequences per second

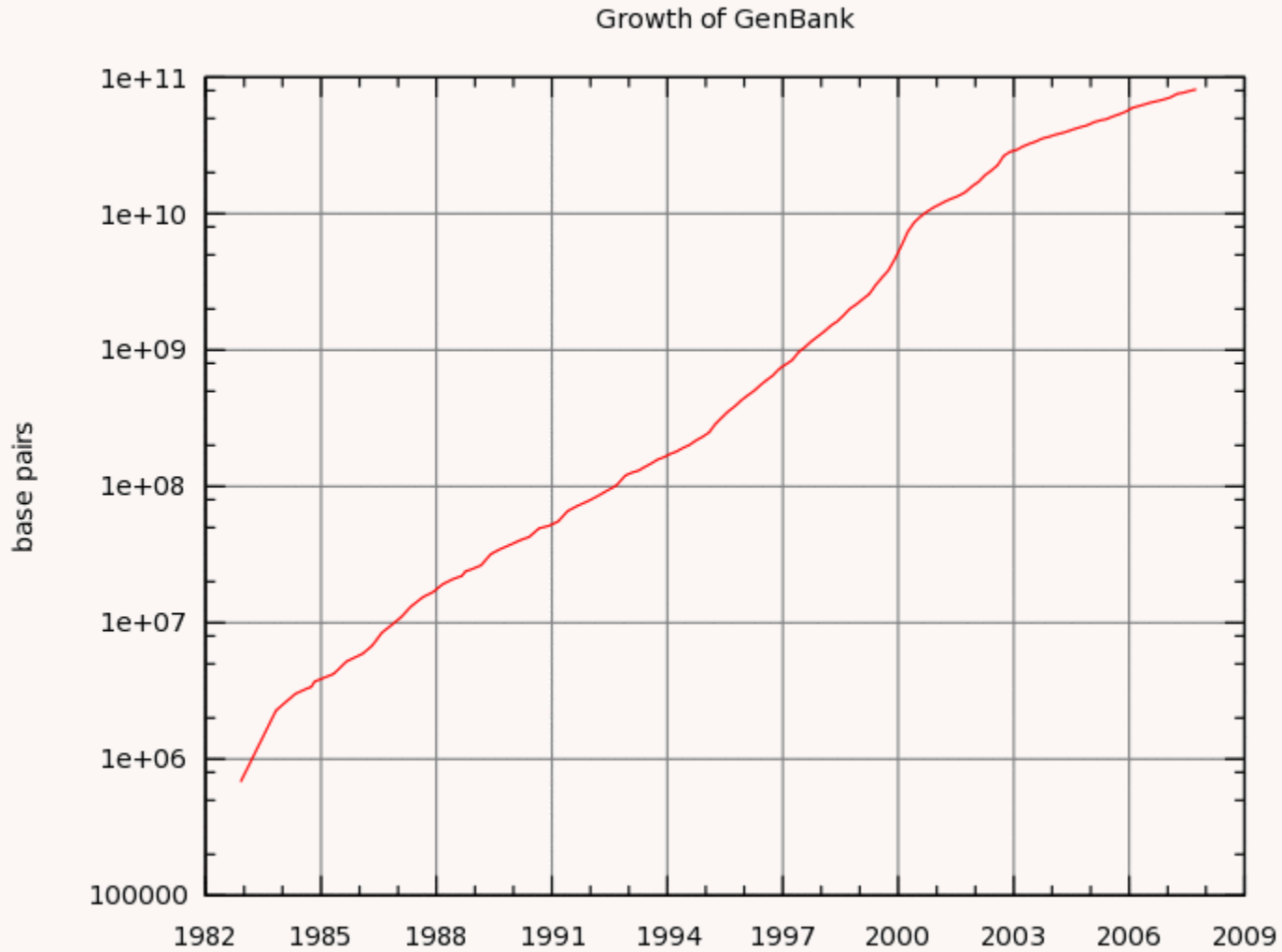
Program	Length	12 core 2.60GHz CPU	GT 730 £53.89	2 K20	K80	GCAT accuracy
BWA	36bp	1900				
	100bp	4500				98.91%
<u>Old Barracuda</u> BWA	36bp		1.7	2.8	3.4	
	100bp		0.4	1.9	2.6	97.49%
<u>New Barracuda</u> BWA	36bp		4.0	6.8	10.5	
	100bp		0.5	2.0	2.8	98.43%
GI Improvement (release code)	36bp		2.32	2.43	3.07	
	100bp		1.13	1.00	1.09	1.6

- Twin GPUs work on each of paired ends
- GT730 estimated as if two in use

Each DNA end with dedicated GPU




“Moore’s Law” in Sequences



The Genetic Programming Bibliography

<http://www.cs.bham.ac.uk/~wbl/biblio/>

10617 references

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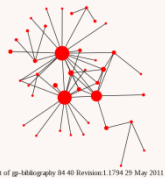
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