Multi-threaded Memory Efficient Crossover in C++
for Generational Genetic Programming

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Abstract
C++ code snippets from a multi-core parallel memory-efficient crossover for genetic programming are given. They may be adapted for separate generation evolutionary algorithms where large chromosomes or small RAM require no more than $M + 2 \times n_{threads}$ simultaneously active individuals.

Figure 1: In generational schemes (e.g. $\mu, \mu$) the current population (on the left) is completely replaced by the next population (on the right). The area of red dots is proportional to the number of children it will be a parent of in the next generation. Small white dots are infertile. We describe how to avoid simultaneously storing both populations.

1 Background
It has been known for a long time that in conventional two parent genetic programming [2, 14] only $M + 2$ individuals are required for non-overlapping generations of $M$ trees [3, pages 1044-1045]. Indeed this is true of other forms of GP [12, 13, 11] and generational Genetic Algorithms and Evolutionary Computation in general. Nonetheless the widespread availability of large RAM computers and compact coding of individual chromosomes seems to have led to the $M + 2$ limit being forgotten and the widespread use of inefficient computer implementations, e.g. [7], with separate new and old populations, each requiring storage for $M$ individuals. Recent work with enormous trees [5, 8] or large populations [9] has prompted renewed interest in ensuring that generational implementations are as efficient as steady state implementations. (For example, see email discussion on GeneticProgramming@groups.io 5–7 September 2020.)

1 Steady state GA [16], GPs [15], and ($\mu + \lambda$)-ES Evolution Strategies use overlapping generations, Figure 2.
Figure 2: In steady state Evolutionary Algorithms (e.g. \( \mu + 1 \)) parents are selected from the current population, their offspring created and inserted into the current population (red). To keep the population size constant, the same number of individuals (white) are removed from the population. Many strategies are available for selecting parents and for selecting who to remove from the population.

2 Minimal Memory Generational Algorithms

Koza et al. [3] pages 1044-1045] divide the current population into four classes, according to how many children they have: 0, 1, 2, more than 2. The new population is created in this priority order (0, 1, 2, 2+). Our algorithm is slightly simpler. Since GPquick [15]'s crossover creates one child (rather than two), this allows the “2” and “more than 2” classes to be combined into a class “two or more” (2+). We then follow [3] pages 1044-1045], except (to allow crossovers in parallel) we allocate up to two free slots per thread (rather than an extra two).

At the start of the new generation, the parent population are assigned into classes 0, 1 and 2+. All the parents without children (class 0) are deleted. The children to be created are assigned into class 1 or 2+, according to the minimum class of their (two) parents. I.e. if either parent is in class 1, the new child is placed in class 1, otherwise class 2+. With rapid parallel fitness evaluation, the cost of crossover can be significant, therefore both crossover and fitness evaluation are done by parallel threads [6]. This means the remaining operations are also done in parallel.

Creation and testing of new individuals then starts with the class 1 individuals. Each time a new individual has been created, it is removed from the data structures for both its parents. If it has a class 1 parent, removing it will mean that that parent now no longer has any children to be processed and so is deleted. Note this can be done before starting fitness evaluation of the child. Removing it from a class 2+ parent, may mean the parent still has two or more children to be processed, so it stays in class 2+ or it may now only have one child to be created, in which case the child is moved to class 1. Class 1 children (i.e. with one or more class 1 parent) are created before those with two class 2+ parents.

The amount of memory used in a particular multi-threaded run is between \( M + 1 \) and \( M + 2 \times n \) threads, and depends on the exact order of operations. The assignment of individuals to threads and the scheduling of those threads typically varies, and so there can be variations in memory usage between otherwise identical runs.
3 C++ pthreads Implementation

Our implementation is aimed at improving memory efficiency of extended runs (weeks) with small populations 500–4000 with tournament selection (7), crossover and trees of a billion nodes, on multi-core parallel compute servers with modest RAM memory (< 1TB). Thus the implementation must support parallel evaluation. Secondly, although our implementation should be widely applicable, this environment lead to various design choices.

3.1 Reusing expr Buffers

In extended runs, where GP trees are allowed to bloat memory consumption is dominated by the space required to store the trees. Since we are starting from a mature C++ code base [6], we only optimise the expr buffers used to store the trees. That is, although we could minimise the number of active individuals (chrome) simultaneously in use, for simplicity and minimising impact on the existing code, we retain separate pop and newpop data structures and concentrate upon expr. (The chrome data structures hold accounting information and, in our use case, are tiny compared to the trees.)

Originally GPquick allocated each chrome and expr buffer as it was created and removed it when the chrome was deleted. Although GNU C++ fully supports multi-threaded dynamic memory allocation and de-allocation, in practice we have found with multiple active threads this comes with a high overhead.

New routine init_exprs (see Appendix A) creates and initialises an array of $M + 2 \times nthreads$ pointers to hold addresses for expr buffers and a free chain linking them all. In a multi-threaded context, these must be protected by a synchronisation lock. get_expr gives the next free expr buffer to its calling chrome. If the chosen expr buffer has not yet been allocated get_expr creates it. (Note all expr buffer are fixed length of $pMaxExpr$ bytes.) In order to allow free_expr to return the expr buffer to the free chain without searching, get_expr also records which expr buffer chrome has been given in the new chrome field expr_id. Note once an expr buffer has been allocated by C++ from the heap it is never returned to the heap. Instead get_expr and free_expr allow it to be reused in each generation.

3.2 Few Children per Parent

In many evolutionary systems the populations tend to converge so that the breeding population (i.e. the existing individuals who will give rise to children) is a sizable fraction (e.g. 30%) of the whole population. Meaning, typically each only has a few children, (e.g. on average about five). Therefore the children data structure uses simple linear arrays to hold the identifiers of the children of each parent (Appendix A.2). At first sight this may seem inefficient.

Short linear scans along a simple vector to add/delete may be faster than more complex data structures which avoid search. Although we have not done this, the target hardware supports AVX vector operations, which can perform operations on up to 16 (or even 32) identifiers in one go.

Allocating and initialising each of the children arrays is eased by knowing before each generation starts how many children each parent will have (num_children). Thus each linear array can be easily created of the correct size.

As mentioned in the previous section, in practice new/delete operations to allocate/remove heap data structures may be expensive when done with multiple active threads. (Which is another reason for avoiding some alternative dynamic data structures.) Therefore all children arrays are pre-allocated and initialised in the default single master thread before any of the new population are constructed by crossover (Appendix A.2.1). Similarly they are all de-allocated after the fitness of the new generation has been evaluated. Although the children arrays are different sizes, they are always small, and we have not noticed any problem with heap fragmentation.
### 3.3 Integration with existing pthreads code

#### 3.3.1 Additional master thread code

In generational mode the existing routine `generation_fitness` (Appendix A.2.1) is used to sort parents and to be created children into class 0, 1 and 2+ (as described in Section 2). After deleting all parents without children (class 0), `generation_fitness` creates `nthreads`. After the threads have all have finished, it removes the `children` arrays. Notice the `children` arrays are allocated from the heap and returned to it, by conventional (non-parallel) code.

As before, `generation_fitness` also removes all the parent `chrome` and switches to `newpop`. As mentioned in Section 3.1, the `chrome` data structures are tiny compared to the space needed to store their trees (i.e. `expr`). Therefore, to limit impact on the existing code, we only minimise the number of `expr` buffers.

#### 3.3.2 Additions to the parallel crossover and fitness evaluations code

The existing `thread_fitness` function (Appendix A.2.3) is executed separately by each of `nthreads`. It consists of a loop, which takes the next unevaluated new child, created it by crossover, and evaluates its fitness. It then goes to the top of the loop to find the next member of the new generation to process. It continues looping until it or the other threads have processed everyone.

The principle changes are:

- Use `chainhd1` and `chainhd2` to process the new population in class priority order (rather than just numerical order).
- Use `get_expr` to allocate space for the new tree (Section 3.1 and Appendix A.1).
- Use functions `remchild` and `move21` to update class 0, 1 and 2+ information (Section 2 Appendix A.2.4).

  - `remchild` is used to remove the new individual from the `children` arrays used by its two parents (`Mum` and `Dad`) after it has been created by crossover (but potentially before fitness evaluation). Note due to multi threading the classes may not be the same as when the child was selected to be processed by the current thread. (Even with a single thread this can also be true of the second call to `remchild`.) Similarly due to potential self-crossover (i.e. overlapping parents), `remchild` must only remove one instance from the `children` array. Since `remchild` is already going to process most of each `children` array, it is a convenient place to see how many children remain to be processed. This is returned to `thread_fitness`. Should there be only one child left for this parent, its id is past via the `last` argument so that it is available to the `move21` function.

  - The `move21` function (Section A.2.4) is actually simple, but the listing is long as the implementation contains extensive sanity checks of the class 1 and class 2+ chains. `move21` removes the indicated parent from the class 2+ chain and then places it at the head of the class 1 chain. Since the parent can be arbitrary it must be removed from the class 2+ chain cleanly. This is implemented using a bidirectional chain (i.e. with both `forw` and `back` pointers). In contrast it can be inserted at the start of the class 1 chain (via `chainhd1`, and so becomes the next item to process). Thus the class 1 chain is not bidirectional and its `back` pointers are not maintained.

As mentioned above, `move21` must deal with cases where the child has already been removed from class 2+. `move21` uses the array `status` (values 0, 1 and 2, meaning class 0, 1 or 2+) to avoid scanning the class 2+ chain. (Also a check is needed that the child is not the one being processed. It is convenient to place that check in `move21`.)

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Figure 3: Example generational GP run on 8 core i7-4790 3.60GHz CPU with 31.2GB of memory. The new efficient handling of memory enables the run to continue 3.5 times as long as would have been possible previously (shown in black). Notice with the earlier limit, the population bloats, whereas the new code (colour, after 11 hours) shows GP gives more interesting dynamics if able to run for longer. The run is terminated after generation 71248 when GP occupies 97.8% of system memory having processed the equivalent of $2.61 \times 10^{16}$ GP opcodes in 37 hours 13 minutes (195 Giga GPop/s, cf. [4, Table 7], [6, Table 1]). Notice although GPquick uses a fixed number (516) of fixed length buffers (3.2 x $10^8$ bytes) to hold the population, the Unix process memory (solid red line) tracks ahead of the memory used to store the trees and is seldom reduced when the trees become smaller (lower, dashed blue, line). Note size of largest tree (purple dots or crosses ×) is rescaled by 516 to put on same scale as average tree (dashed blue line). When not gathering details statistics, all but 0.14% of run time is used by crossover and fitness evaluation (i.e. in the 8 parallel threads). However, despite having 500 trees to evaluate with 8 threads, variation in fitness times leads to fast threads being idle waiting on the longest duration thread. In this run this leads to losing 91.9% of a core. I.e. on average our generational GPquick effectively used only 7.08 cores in this run.
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A GPquick C++ Code Snippets. chrome.cxx Revision: 1.262

Standard C++ conditional compilation `#ifndef NDEBUG` and `assert()` are used only during development and are disabled when compiled with `-O3 -DNDEBUG`.

http://www.cs.ucl.ac.uk/staff/W.Langdon/ftp/gp-code/efficient_memory/

A.1 expr buffers

```cpp
void Pop::init_exprs(const int nexpr){
    assert(thispop==NULL);
    thispop = this;
    assert(chain==NULL);
    const int n = nexpr+1;
    chain = new int[n]; //leave 0 unused
    exprptr = new nodeptr[n]; //leave 0 unused
    memset(exprptr,0,n*sizeof(node*));
    chain[0] = 0; //be tidy
    for(int i=1;i<nexpr;i++) chain[i] = i+1;
    chain[nexpr] = 0; //end of chain
    chainmax = nexpr; //for debug
    chainhead = 1;
}
```

```cpp
class Pop ...//NB protect with external locks
int used = 0; //only for performance monitoring
int max_used = 0; //only for performance monitoring

void Pop::get_expr(Chrome* chrome){
    assert(chainhead<=chainmax);
    if(chainhead==0) {
        cout<<"ERROR ran out of expr buffers "
            <<popsize<<" "<<chainmax<<" "<<chainhead
            <<" pThreads: "<<params->params[pThreads]<<endl;
        exit(1);
    }
    if(exprptr[chainhead]==0){
        exprptr[chainhead] = new node[params->params[pMaxExpr]];
    }
    chrome->expr = exprptr[chainhead];
    chrome->expr_id = chainhead;
    chainhead = chain[chainhead];
    assert(chainhead==0 || (chainhead>=1 && chainhead<=chainmax));
    used++;
    if(used>max_used){
        max_used = used;
        const int nthreads = params->params[pThreads];
        const int nexpr = popsize + 2*( (nthreads==0)? 1 : nthreads);
        if(nthreads && max_used > nexpr) cout<<"ERROR max_used increased to "
            <<max_used<<endl;
    }
}
```
void Pop::free_expr(Chrome* chrome){
    const int id = chrome->expr_id;
    if(id==0) return; //already freed
    assert(id>=1 && id<=chainmax);
    assert(exprptr[id]!=0);
    assert(chainhead==0 || (chainhead>=1 && chainhead<=chainmax));
    chain[id] = chainhead;
    chainhead = id;
    assert(chainhead==0 || (chainhead>=1 && chainhead<=chainmax));
    used--;
    assert(used>=0);
    chrome->expr_id = 0; //allow free_expr to be called more than once
}

A.2 Tracking Children to be Created by Crossover and Freeing their Parents

Note whilst expr buffers uses 0 to denote an invalid value, e.g. end of chain, the following code uses -1.

int* forw = NULL; //valid 0..popsize-1
int* back = NULL; //valid 0..popsize-1, only maintained for chain2
int** children = NULL; //popsize NULL or pointer to num_children int, -1 or 0..popsize-1
int* status = NULL; //0, 1 or 2
int chainhd1 = -1; //valid 0..popsize-1
int chainhd2 = -1; //valid 0..popsize-1

A.2.1 generation_fitness

Fragment of code in master thread used at the start of each generation (except the first random population) in function generation_fitness.

if(DoCross) { //100% crossover on later generations
    if(forw == NULL) forw = new int[popsize];
    if(back == NULL) back = new int[popsize];
    if(status == NULL) status = new int[popsize];
    if(children == NULL) children = new int*[popsize];
    #ifndef NDEBUG
    memset(forw, 0x7f,popsize*sizeof(int));
    memset(back, 0x7f,popsize*sizeof(int));
    memset(status, 0xff,popsize*sizeof(int));
    #endif
    memset(children,0,popsize*sizeof(int));
    int last1 = -1;
    int last2 = -1;
    chainhd1 = -1;
    chainhd2 = -1;
    for(int s=0;s<popsize;s++) {
        assert(newpop[s]->mum.birth >= 0);
        assert(newpop[s]->dad.birth >= 0);
        const int Mum = newpop[s]->mum.birth % popsize;
        const int Dad = newpop[s]->dad.birth % popsize;
        ...
const Chrome* mum = pop[Mum];
const Chrome* dad = pop[Dad];
assert(mum->num_children>0);
assert(dad->num_children>0);
if(mum->num_children==1 || dad->num_children==1) {
    append(s, last1, chainhd1);
    status[s] = 1;
} else {
    append(s, last2, chainhd2);
    status[s] = 2;
}
addchild(Mum,mum->num_children,s);
addchild(Dad,dad->num_children,s);
}

for(int s=0;s<popsize;s++) {
    if(pop[s]->num_children==0) {delete pop[s]; pop[s] = NULL;}
}
}

A.2.2 Functions used by generation_fitness

inline void append(const int s, int& last, int& chainhd) {
    const int popsize = thispop->popsize;
    assert(s>=0 && s < popsize);
    if(last != -1) {
        assert(forw[last] == -1); forw[last] = s; }
    assert( forw[s]  == 0x7f7f7f7f); forw[s] = -1;
    assert( back[s]  == 0x7f7f7f7f); back[s] = last;
    last = s;
    if(chainhd == -1) chainhd = s;
}

inline void addchild(const int P,const int num_children,const int s) {
    //use linear search assuming num_children is small
    const int popsize = thispop->popsize;
    assert(P>=0 && P < popsize);
    assert(s>=0 && s < popsize);
    //if(!(num_children > 0 && num_children < 20)) cout<<"num_children "<<num_children<<endl;
    if(children[P]==NULL) {
        children[P] = new int[num_children];
        memset(children[P],0xff,num_children*sizeof(int));
    }
    int i=0;
    for(;i<num_children;i++){
        if(children[P][i] == -1){children[P][i]=s;break;}
    }
    assert(i < num_children);
    assert(children[P][i]==s);
}
A.2.3 Multi-threaded code, i.e. thread_fitness

Fragments of multi-threaded code used during crossover and fitness evaluation in each generation (except the first) in function thread_fitness.

Allocate new child i for the thread to work on. Choose i from class 1 if any, otherwise from class 2+.
If both classes are empty, there is no more work, so stop the thread.

```
Chrome* newguy;
{
    const int e = pthread_mutex_lock(&mutex); assert(e==0);
}
if(DoCross) { //100% crossover on later generations
    int i = -1;
    if(  chainhd1 != -1) {
        i = chainhd1;
        chainhd1 = forw[i];
    } else if(chainhd2 != -1) {
        i = chainhd2;
        chainhd2 = forw[i];
    }
    if(i == -1) {
        {
            const int e = pthread_mutex_unlock(&mutex); assert(e==0);
        }
        break;
    }
    assert(status[i]==1 || status[i]==2);
    status[i] = 0; //make sure no other thread tries to process i
    newguy = thispop->newpop[i];
    newguy->thread = my_id;
    assert(newguy->expr == NULL);
    thispop->get_expr(newguy);
    {
        const int e = pthread_mutex_unlock(&mutex); assert(e==0);
    }
}
```

Do crossover. Reading from Mum and Dad writing new child into newguy.

After crossover, unless doing incremental fitness, now ok to remove newguy from both its parents. If either parent was in class 2+ but now only has one child left to be processed, the parent is moved to class 1. If either parent now has no children left to process, it is deleted. Note freeing mutex to allow crossovers to be done in parallel means other threads may have already processed other children with the same parents, so, for example, a parent may no longer be in class 2+ when move21 is called to move it from 2+ to 1.

```
{
    const int e = pthread_mutex_lock(&mutex); assert(e==0);
}
int last1, last2;
const int nchild1 = remchild(Mum,mum->num_children,i,last1);
const int nchild2 = remchild(Dad,dad->num_children,i,last2);
if(nchild1 == 1) move21(i,last1);
if(nchild2 == 1) move21(i,last2);
if(nchild1 == 0) {
    mum->num_children = 0;
    thispop->free_expr(mum);
}
if(nchild2 == 0) {
    dad->num_children = 0;
    thispop->free_expr(dad);
}
{
    const int e = pthread_mutex_unlock(&mutex); assert(e==0);
}
```

Do fitness evaluation for newguy and then loop to top of function thread_fitness to see if there is any more work to be done.
A.2.4 Multi-threaded Functions used by thread_fitness

```c
inline int remchild(const int P, const int num_children, const int s, int& last) {
    // use linear search assuming num_children is small
    const int popsize = thispop->popsize;
    assert(P >= 0 && P < popsize);
    assert(s >= 0 && s < popsize);
    int S = s;
    int nchild = 0;
    int ok = 0;
    for(int i = 0; i < num_children; i++) {
        assert(children[P][i] >= -1 && children[P][i] < popsize);
        if(children[P][i] == S) {
            children[P][i] = -1;
            ok++;
            S = -2;
        }
        if(children[P][i] != -1) {
            last = children[P][i];
            nchild++;
        }
    }
    assert(ok == 1);
    if(nchild != 1) last = -1; // be tidy
    return nchild;
}

inline void move21(const int active, const int s) {
    if(active == s) return; // ignore
    if(status[s] != 2) return; // already processed
    // remove s from chain2
    status[s] = 1;
    const int b = back[s];
    const int f = forw[s];
    if(chainhd2 == s) chainhd2 = f;
    forw[s] = -1;
    back[s] = -1;
    if(b != -1) forw[b] = f;
    if(f != -1) back[f] = b;

    // Insert s at head of chain1
    forw[s] = chainhd1;
    chainhd1 = s;
} // end move21
```