

# Multiscale modeling

## Monte Carlo static recrystallization

All my code can be found on Git repository at <https://github.com/vonProteus/MultiscaleModelling-SimpleGrainGrowthCA>

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# My Code

In my code there is possibility to do static recrystallization with Monte Carlo method. The Monte Carlo method is very interesting because it uses random numbers to get meaningful and realistic results. Code which performs this is very simple and looks like this.

```
self.neighborsType = MoorNeighborhood;
NSMutableArray* toGo = [NSMutableArray array];
for (NSInteger a = 0; a < y; ++a) {
    for (NSInteger b = 0; b < x; ++b) {
        MKCell* currentCell = [self getX:b
                                   Y:a];

        if (currentCell.isOnBorder) {
            [toGo addObject:currentCell];
        }
    }
}

while ([toGo count] > 0) {
    MKCell* cell = [toGo objectAtIndex:arc4random() % [toGo count]];
    if (cell.grainId > 0) {
        NSMutableSet* neighbors = [self
            getAllNeighborsWhoCanGrowForX:cell.coordinateX
                                   andY:cell.coordinateY];

        CGFloat energy = cell.energy;
        CGFloat newEnergy = 0;

        MKCell* newCell = [[neighbors allObjects] objectAtIndex:arc4random() %
            [neighbors count]];
        NSInteger newId = newCell.grainId;

        for (MKCell* neighbor in neighbors) {
            energy += neighbor.energy;
            newEnergy += neighbor.energy;
        }

        if (newEnergy < energy) {
            cell.grainId = newId;
            cell.energy = 0;
            cell.willGrow = YES;
            [[self getPrevX:cell.coordinateX
                                   Y:cell.coordinateY] getAllFrom:cell];
            ++changes;
        }
    }
    [toGo removeObject:cell];
}
```

In the first block we only get cells that are on the border. This considerably reduces time of computation.

Then we randomly get one cell from the border and start counting energy of a cell before change and after. If the energy after change is lower then we commit the change, otherwise we do not change the cell

# Computation on Zeus

I submitted 24 tasks of which 8 never started, 6 failed, 4 finished with exit code 1, and 6 finish normally. I was waiting for 24H before starting writing this report so i think that i gave enough time to the queued task.

My goal was to run two types of simulation grain growth and grain growth with recrystallization with every type of neighborhood supported by MCMicro (hex, moore, neumann and penta). Each simulation I submitted with wall time of 1H and 1GB limit of Ram. Each simulation was submitted 3 times with different number of cores. All tasks were submitted in parallel mode.

This is how the results look like

ID	Name	Application	Appli...	Main File	Status	Work dir	Resource	Submission time	Start time	End time	Sweep idx
d6...db4	hex.mcmmicro	MCMicro		hex.mcmmicro	Failed	/Users/teak/Desktop/r2/gg/hex/1	Zeus (Cyfronet)	2014.06...18:46:14	2014.06.07 18:48:17	2014.06.07 18:48:17	
fb4...2da	hex.mcmmicro	MCMicro		hex.mcmmicro	Failed	/Users/teak/Desktop/r2/gg/hex/12	Zeus (Cyfronet)	2014.06...18:46:51	2014.06.07 18:48:09	2014.06.07 18:48:17	
08...71f	hex.mcmmicro	MCMicro		hex.mcmmicro	Queued	/Users/teak/Desktop/r2/gg/hex/24	Zeus (Cyfronet)	2014.06...18:47:04			
da1...78f	moore.mcmmicro	MCMicro		moore.mcmmicro	Finished	/Users/teak/Desktop/r2/gg/moore/1	Zeus (Cyfronet)	2014.06...15:21:30	2014.06.07 15:25:27	2014.06.07 15:26:52	
21...585	moore.mcmmicro	MCMicro		moore.mcmmicro	Failed	/Users/teak/Desktop/r2/gg/moore/12	Zeus (Cyfronet)	2014.06...15:22:41	2014.06.07 15:55:24	2014.06.07 16:25:43	
3a...4b4	moore.mcmmicro	MCMicro		moore.mcmmicro	Queued	/Users/teak/Desktop/r2/gg/moore/24	Zeus (Cyfronet)	2014.06...15:23:06			
19...99b	numan.mcmmicro	MCMicro		numan.mcmmicro	Finished	/Users/teak/Desktop/r2/gg/numann/1	Zeus (Cyfronet)	2014.06...15:31:05	2014.06.07 15:32:28	2014.06.07 15:36:32	
31...9ab	numan.mcmmicro	MCMicro		numan.mcmmicro	Failed	/Users/teak/Desktop/r2/gg/numann/12	Zeus (Cyfronet)	2014.06...15:31:29	2014.06.07 15:58:23	2014.06.07 16:32:50	
5d...24b	numan.mcmmicro	MCMicro		numan.mcmmicro	Queued	/Users/teak/Desktop/r2/gg/numann/24	Zeus (Cyfronet)	2014.06...15:32:13			
03...630	pent.mcmmicro	MCMicro		pent.mcmmicro	Finished	/Users/teak/Desktop/r2/gg/pent/1	Zeus (Cyfronet)	2014.06...15:34:59	2014.06.07 15:36:39	2014.06.07 15:40:47	
1c...342	pent.mcmmicro	MCMicro		pent.mcmmicro	Failed	/Users/teak/Desktop/r2/gg/pent/12	Zeus (Cyfronet)	2014.06...15:35:24	2014.06.07 15:55:25	2014.06.07 16:39:14	
40...9a6	pent.mcmmicro	MCMicro		pent.mcmmicro	Queued	/Users/teak/Desktop/r2/gg/pent/24	Zeus (Cyfronet)	2014.06...15:36:00			
92...1ec	hex.mcmmicro	MCMicro		hex.mcmmicro	Failed	/Users/teak/Desktop/r2/gg+srx/hex/1	Zeus (Cyfronet)	2014.06...15:37:22	2014.06.07 15:38:24	2014.06.07 15:38:30	
c3...9b0	hex.mcmmicro	MCMicro		hex.mcmmicro	Finish...code=1	/Users/teak/Desktop/r2/gg+srx/hex/12	Zeus (Cyfronet)	2014.06...15:38:11	2014.06.07 15:38:26	2014.06.07 15:38:31	
de...d40	hex.mcmmicro	MCMicro		hex.mcmmicro	Queued	/Users/teak/Desktop/r2/gg+srx/hex/24	Zeus (Cyfronet)	2014.06...15:38:38			
20...8ba	moore.mcmmicro	MCMicro		moore.mcmmicro	Finished	/Users/teak/Desktop/r2/gg+srx/moore/1	Zeus (Cyfronet)	2014.06...15:39:44	2014.06.07 15:55:26	2014.06.07 16:00:43	
3d...ddf	moore.mcmmicro	MCMicro		moore.mcmmicro	Finish...code=1	/Users/teak/Desktop/r2/gg+srx/moore/12	Zeus (Cyfronet)	2014.06...15:40:13	2014.06.07 15:40:29	2014.06.07 15:40:29	
56...213	moore.mcmmicro	MCMicro		moore.mcmmicro	Queued	/Users/teak/Desktop/r2/gg+srx/moore/24	Zeus (Cyfronet)	2014.06...15:40:38			
8d...7e5	numan.mcmmicro	MCMicro		numan.mcmmicro	Finished	/Users/teak/Desktop/r2/gg+srx/numann/1	Zeus (Cyfronet)	2014.06...15:41:33	2014.06.07 15:55:26	2014.06.07 15:59:41	
a31...f53	numan.mcmmicro	MCMicro		numan.mcmmicro	Finish...code=1	/Users/teak/Desktop/r2/gg+srx/numann/12	Zeus (Cyfronet)	2014.06...15:41:55	2014.06.07 15:42:25	2014.06.07 15:42:31	
d4...b5b	numan.mcmmicro	MCMicro		numan.mcmmicro	Queued	/Users/teak/Desktop/r2/gg+srx/numann/24	Zeus (Cyfronet)	2014.06...15:42:44			
ef1...05d	pent.mcmmicro	MCMicro		pent.mcmmicro	Finished	/Users/teak/Desktop/r2/gg+srx/pent/1	Zeus (Cyfronet)	2014.06...15:43:11	2014.06.07 15:55:26	2014.06.07 16:01:04	
0c...d38	pent.mcmmicro	MCMicro		pent.mcmmicro	Finish...code=1	/Users/teak/Desktop/r2/gg+srx/pent/12	Zeus (Cyfronet)	2014.06...15:43:40	2014.06.07 15:44:29	2014.06.07 15:44:29	
22...a23	pent.mcmmicro	MCMicro		pent.mcmmicro	Queued	/Users/teak/Desktop/r2/gg+srx/pent/24	Zeus (Cyfronet)	2014.06...15:44:02			

## Grain Growth

	1 Node 1 Core	1 Node 12 Core	1 Node 24 Core
<b>Hex</b>	Failed	Failed	Queued
<b>Moore</b>	Finished (229s)	Failed	Queued
<b>Numan</b>	Finished (183s)	Failed	Queued
<b>Penta</b>	Finished (206s)	Failed	Queued

## Grain Growth + SRX

	1 Node 1 Core	1 Node 12 Core	1 Node 24 Core
<b>Hex</b>	Failed	Failed [Exit code =1]	Queued
<b>Moore</b>	Finished (842s)	Failed [Exit code =1]	Queued
<b>Numan</b>	Finished (635s)	Failed [Exit code =1]	Queued
<b>Penta</b>	Finished (674s)	Failed [Exit code =1]	Queued

## Detailed results

All results and input files can be found here <https://tywin.photep.net/owncloud/public.php?service=files&t=4d6b9a29a3b88266706bb4b26c2cdfca>

## Grain Growth HEX

output from 1 node 1 core

```
'compilers/gcc/4.8.2' load complete.
'tools/openmpi/1.6.5-gnu-4.8.2-ib' load complete.
'plgrid/apps/mcmicro/1.0' load complete.
1
[n0141-g5l.zeus:01191] mca: base: component_find: unable to open /software/
local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/openmpi/mca_btl_ofud:
librdmacm.so.1: cannot open shared object file: No such file or directory
(ignored)
[n0141-g5l.zeus:01191] mca: base: component_find: unable to open /software/
local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/openmpi/mca_btl_openib:
librdmacm.so.1: cannot open shared object file: No such file or directory
(ignored)
[n0141-g5l.zeus:01191] mca: base: component_find: unable to open /software/
local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/openmpi/mca_mtl_psm:
libpsm_infinipath.so.1: cannot open shared object file: No such file or
directory (ignored)
1200 1200
My rank: 0 xSize: 1200 ySize: 1200 zSize: 1
My rank: 0 Grain Growth simulation start
[n0141-g5l:01191] *** Process received signal ***
[n0141-g5l:01191] Signal: Segmentation fault (11)
[n0141-g5l:01191] Signal code: Address not mapped (1)
[n0141-g5l:01191] Failing at address: 0x10
[n0141-g5l:01191] [ 0] /lib64/libpthread.so.0(+0xf710) [0x2b766d9be710]
[n0141-g5l:01191] [ 1] MCMicro_MPI(_ZN12Neighborhood17getneighboursSizeEv+0)
[0x428c00]
[n0141-g5l:01191] [ 2] MCMicro_MPI(_ZN5Space22initializeNeighborhoodEi+0x1c)
[0x4151bc]
[n0141-g5l:01191] [ 3]
MCMicro_MPI(_ZN13McGrainGrowthC1EP5Spaceiidi18BoundaryConditions+0x102)
[0x422d02]
[n0141-g5l:01191] [ 4] MCMicro_MPI(main+0x6f6) [0x414b46]
[n0141-g5l:01191] [ 5] /lib64/libc.so.6(__libc_start_main+0xfd)
[0x2b766d9bead1d]
[n0141-g5l:01191] [ 6] MCMicro_MPI() [0x4117bd]
[n0141-g5l:01191] *** End of error message ***
-----
mpirun noticed that process rank 0 with PID 1191 on node n0141-g5l.zeus
exited on signal 11 (Segmentation fault).
-----
```

output from 1 node 12 core

```
'compilers/gcc/4.8.2' load complete.
'tools/openmpi/1.6.5-gnu-4.8.2-ib' load complete.
'plgrid/apps/mcmicro/1.0' load complete.
1
1
1
1
1
1
1
1
1
1
1
1
1
1
1
1
My rank: 9 xSize: 100 ySize: 1200 zSize: 1
My rank: 3 xSize: 100 ySize: 1200 zSize: 1
My rank: 4 xSize: 100 ySize: 1200 zSize: 1
My rank: 10 xSize: 100 ySize: 1200 zSize: 1
My rank: 8 xSize: 100 ySize: 1200 zSize: 1
My rank: 1 xSize: 100 ySize: 1200 zSize: 1
My rank: 2 xSize: 100 ySize: 1200 zSize: 1
1200 1200
My rank: 0 xSize: 100 ySize: 1200 zSize: 1
My rank: 5 xSize: 100 ySize: 1200 zSize: 1
My rank: 6 xSize: 100 ySize: 1200 zSize: 1
My rank: 7 xSize: 100 ySize: 1200 zSize: 1
My rank: 11 xSize: 100 ySize: 1200 zSize: 1
-----
mpixec noticed that process rank 0 with PID 26437 on node n0518-g7x.zeus
exited on signal 11 (Segmentation fault).
-----
```

Both times occurred segmentation fault as you can see

## Grain Growth MOORE

For 1 node 1 core the computation was successful and took 229s.  
For 1 node 12 cores an error occurred

13 s.  
node: 2 MCS: 100

13 s.  
node: 10 MCS: 100

13 s.  
node: 1 MCS: 100

13 s.  
node: 11 MCS: 100

13 s.  
node: 0 MCS: 100

13 s.  
Wszystkie wezly skonczyly obliczenia

```
MCMicro_MPI:16844 terminated with signal 11 at PC=2b7023edcbca
SP=7fff0225e390. Backtrace:
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(opal_memory_ptmalloc2_int_free+0x27a) [0x2b7023edcbca]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(opal_memory_ptmalloc2_free+0xd3) [0x2b7023edd0f3]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(+0x4c3e9) [0x2b7023e303e9]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(mca_pml_base_close+0x41) [0x2b7023e7efe1]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(ompi_mpi_finalize+0x2e4) [0x2b7023e46c74]
MCMicro_MPI(main+0x59f) [0x4149ef]
/lib64/libc.so.6(__libc_start_main+0xfd) [0x2b70254bcd1d]
MCMicro_MPI[0x4117bd]
```

Only the end of the log is shown.

## Grain Growth NUMAN

For 1 node 1 core the computation was successful and took 183s.

For 1 node 12 cores an error occurred

13 s.  
node: 4 MCS: 100

13 s.  
node: 6 MCS: 100

13 s.  
node: 5 MCS: 100

13 s.  
Wszystkie wezly skonczyly obliczenia

```
MCMicro_MPI:32531 terminated with signal 11 at PC=2b2c82d3cbca
SP=7fff05db7b30. Backtrace:
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(opal_memory_ptmalloc2_int_free+0x27a)[0x2b2c82d3cbca]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(opal_memory_ptmalloc2_free+0xd3)[0x2b2c82d3d0f3]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(+0x4c3e9)[0x2b2c82c903e9]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(mca_pml_base_close+0x41)[0x2b2c82cdefe1]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(ompi_mpi_finalize+0x2e4)[0x2b2c82ca6c74]
MCMicro_MPI(main+0x59f)[0x4149ef]
/lib64/libc.so.6(__libc_start_main+0xfd)[0x2b2c8431cd1d]
MCMicro_MPI[0x4117bd]
QCG-ERROR: Job killed: either user action or resources (e.g. walltime)
exceeded
```

Only the end of the log is shown.

## Grain Growth PENTA

For 1 node 1 core the computation was successful and took 206s.

For 1 node 12 cores an error occurred

13 s.  
node: 9 MCS: 100

13 s.  
node: 6 MCS: 100

13 s.  
node: 8 MCS: 100

13 s.  
node: 7 MCS: 100

13 s.  
Wszystkie wezly skonczyly obliczenia

```
MCMicro_MPI:30963 terminated with signal 11 at PC=2b70223cdbca
SP=7fff22f8f2f0. Backtrace:
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(opal_memory_ptmalloc2_int_free+0x27a) [0x2b70223cdbca]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(opal_memory_ptmalloc2_free+0xd3) [0x2b70223ce0f3]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(+0x4c3e9) [0x2b70223213e9]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(mca_pml_base_close+0x41) [0x2b702236ffe1]
/software/local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/libmpi.so.
1(ompi_mpi_finalize+0x2e4) [0x2b7022337c74]
MCMicro_MPI(main+0x59f) [0x4149ef]
/lib64/libc.so.6(__libc_start_main+0xfd) [0x2b70239add1d]
MCMicro_MPI[0x4117bd]
```

Only the end of the log is shown.



## Grain Growth with Static Recrystallization HEX

output from 1 node 1 core

```
'compilers/gcc/4.8.2' load complete.
'tools/openmpi/1.6.5-gnu-4.8.2-ib' load complete.
'plgrid/apps/mcmicro/1.0' load complete.
3
[n0130-g5l.zeus:29990] mca: base: component_find: unable to open /software/
local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/openmpi/mca_btl_ofud:
librdmacm.so.1: cannot open shared object file: No such file or directory
(ignored)
[n0130-g5l.zeus:29990] mca: base: component_find: unable to open /software/
local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/openmpi/mca_btl_openib:
librdmacm.so.1: cannot open shared object file: No such file or directory
(ignored)
[n0130-g5l.zeus:29990] mca: base: component_find: unable to open /software/
local/el6/COMMON/OpenMPI/1.6.5/ib/gnu/4.8.2/lib/openmpi/mca_mtl_psm:
libpsm_infinipath.so.1: cannot open shared object file: No such file or
directory (ignored)
1200 1200
My rank: 0 xSize: 1200 ySize: 1200 zSize: 1
My rank: 0 Grain Growth simulation start
[n0130-g5l:29990] *** Process received signal ***
[n0130-g5l:29990] Signal: Segmentation fault (11)
[n0130-g5l:29990] Signal code: Address not mapped (1)
[n0130-g5l:29990] Failing at address: 0x10
[n0130-g5l:29990] [ 0] /lib64/libpthread.so.0(+0xf710) [0x2b70a9f58710]
[n0130-g5l:29990] [ 1] MCMicro_MPI(_ZN12Neighborhood17getneighboursSizeEv+0)
[0x428c00]
[n0130-g5l:29990] [ 2] MCMicro_MPI(_ZN5Space22initializeNeighborhoodEi+0x1c)
[0x4151bc]
[n0130-g5l:29990] [ 3]
MCMicro_MPI(_ZN13McGrainGrowthC1EP5Spaceiidiii18BoundaryConditions+0x102)
[0x422d02]
[n0130-g5l:29990] [ 4] MCMicro_MPI(main+0x6f6) [0x414b46]
[n0130-g5l:29990] [ 5] /lib64/libc.so.6(__libc_start_main+0xfd)
[0x2b70aa184d1d]
[n0130-g5l:29990] [ 6] MCMicro_MPI() [0x4117bd]
[n0130-g5l:29990] *** End of error message ***
-----
mpixexec noticed that process rank 0 with PID 29990 on node n0130-g5l.zeus
exited on signal 11 (Segmentation fault).
-----
```

```
'compilers/gcc/4.8.2' load complete.  
'tools/openmpi/1.6.5-gnu-4.8.2-ib' load complete.  
'plgrid/apps/mcmicro/1.0' load complete.  
3  
3  
3  
3  
3  
3  
3  
3  
3  
3  
n0311-g6l: Unable to allocate shared memory for intra-node messaging.  
n0311-g6l: Delete stale shared memory files in /dev/shm.  
n0311-g6l: Unable to allocate shared memory for intra-node messaging.  
n0311-g6l: Delete stale shared memory files in /dev/shm.  
n0311-g6l: Unable to allocate shared memory for intra-node messaging.  
n0311-g6l: Delete stale shared memory files in /dev/shm.  
n0311-g6l: Unable to allocate shared memory for intra-node messaging.  
n0311-g6l: Delete stale shared memory files in /dev/shm.  
n0311-g6l: Unable to allocate shared memory for intra-node messaging.  
n0311-g6l: Delete stale shared memory files in /dev/shm.  
n0311-g6l: Unable to allocate shared memory for intra-node messaging.  
n0311-g6l: Delete stale shared memory files in /dev/shm.  
n0311-g6l: Unable to allocate shared memory for intra-node messaging.  
n0311-g6l: Delete stale shared memory files in /dev/shm.  
n0311-g6l: Unable to allocate shared memory for intra-node messaging.  
n0311-g6l: Delete stale shared memory files in /dev/shm.  
-----  
mpirun has exited due to process rank 7 with PID 23526 on  
node n0311-g6l.zeus exiting improperly. There are two reasons this could  
occur:  
  
1. this process did not call "init" before exiting, but others in  
the job did. This can cause a job to hang indefinitely while it waits  
for all processes to call "init". By rule, if one process calls "init",  
then ALL processes must call "init" prior to termination.  
  
2. this process called "init", but exited without calling "finalize".  
By rule, all processes that call "init" MUST call "finalize" prior to  
exiting or it will be considered an "abnormal termination"  
  
This may have caused other processes in the application to be  
terminated by signals sent by mpirun (as reported here).
```

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## Grain Growth with Static Recrystallization MOORE

For 1 node 1 core the computation was successful and took 842s.

For 1 node 12 cores an error occurred

```
'compilers/gcc/4.8.2' load complete.
'tools/openmpi/1.6.5-gnu-4.8.2-ib' load complete.
'plgrid/apps/mcmicro/1.0' load complete.
3
3
3
3
3
3
3
3
3
3
3
3
3
3
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
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n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
-----
mpiexec has exited due to process rank 1 with PID 23646 on
node n0311-g6l.zeus exiting improperly. There are two reasons this could
occur:

1. this process did not call "init" before exiting, but others in
the job did. This can cause a job to hang indefinitely while it waits
for all processes to call "init". By rule, if one process calls "init",
then ALL processes must call "init" prior to termination.

2. this process called "init", but exited without calling "finalize".
By rule, all processes that call "init" MUST call "finalize" prior to
exiting or it will be considered an "abnormal termination"

This may have caused other processes in the application to be
terminated by signals sent by mpiexec (as reported here).
-----
```

Only the end of the log is shown.

## Grain Growth with Static Recrystallization NUMAN

For 1 node 1 core computation was successful and took 635s.

For 1 node 12 cores error occurred

```
'compilers/gcc/4.8.2' load complete.
'tools/openmpi/1.6.5-gnu-4.8.2-ib' load complete.
'plgrid/apps/mcmicro/1.0' load complete.
3
3
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3
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
-----
mpiexec has exited due to process rank 1 with PID 23768 on
node n0311-g6l.zeus exiting improperly. There are two reasons this could
occur:

1. this process did not call "init" before exiting, but others in
the job did. This can cause a job to hang indefinitely while it waits
for all processes to call "init". By rule, if one process calls "init",
then ALL processes must call "init" prior to termination.

2. this process called "init", but exited without calling "finalize".
By rule, all processes that call "init" MUST call "finalize" prior to
exiting or it will be considered an "abnormal termination"

This may have caused other processes in the application to be
terminated by signals sent by mpiexec (as reported here).
-----
```

## Grain Growth with Static Recrystallization PENTA

For 1 node 1 core the computation was successful and took 674s.

For 1 node 12 cores an error occurred

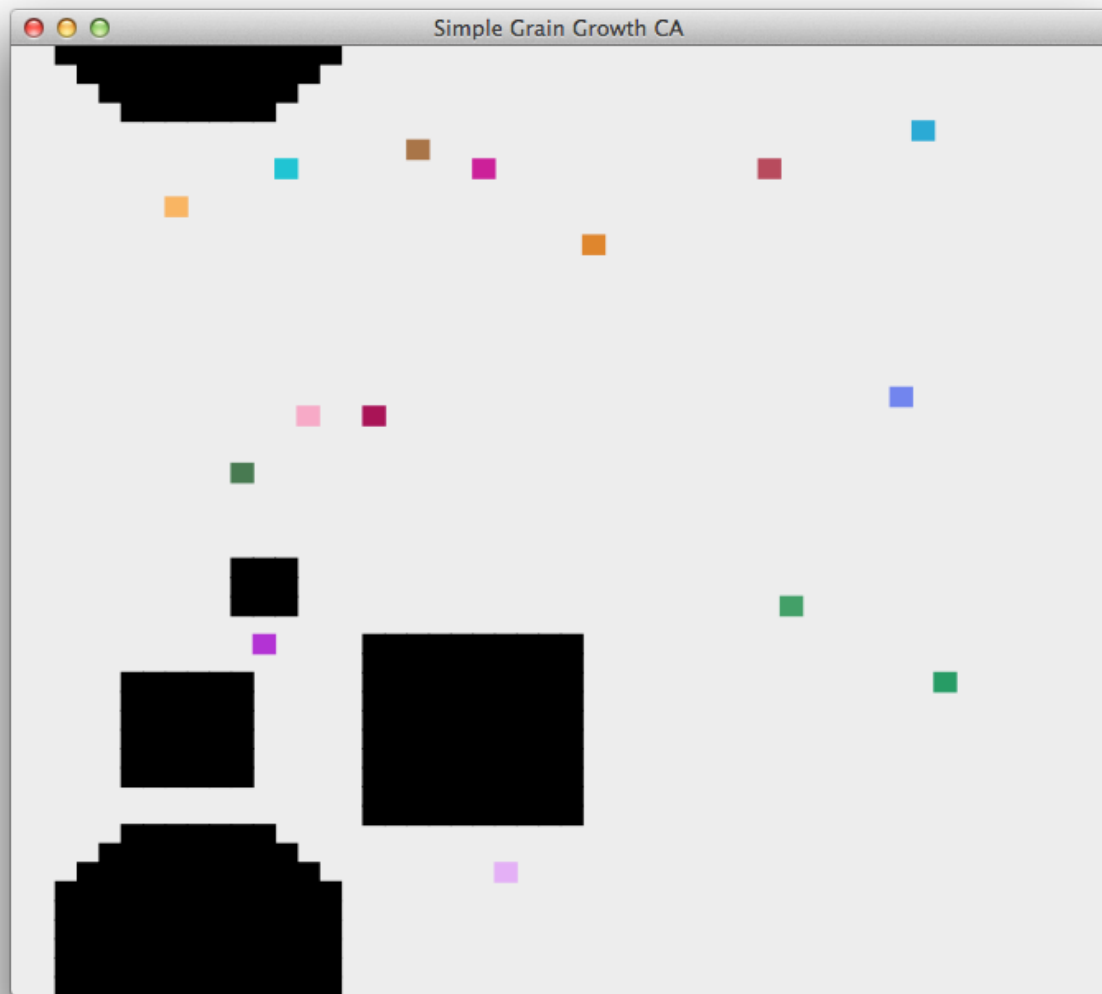
```
'compilers/gcc/4.8.2' load complete.
'tools/openmpi/1.6.5-gnu-4.8.2-ib' load complete.
'plgrid/apps/mcmicro/1.0' load complete.
3
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3
3
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
n0311-g6l: Unable to allocate shared memory for intra-node messaging.
n0311-g6l: Delete stale shared memory files in /dev/shm.
-----
mpirun has exited due to process rank 5 with PID 23892 on
node n0311-g6l.zeus exiting improperly. There are two reasons this could
occur:

1. this process did not call "init" before exiting, but others in
the job did. This can cause a job to hang indefinitely while it waits
for all processes to call "init". By rule, if one process calls "init",
then ALL processes must call "init" prior to termination.

2. this process called "init", but exited without calling "finalize".
By rule, all processes that call "init" MUST call "finalize" prior to
exiting or it will be considered an "abnormal termination"

This may have caused other processes in the application to be
terminated by signals sent by mpirun (as reported here).
-----
```

# Capabilities software



This is how software looks like after launch. As we can see we have some grains nucleons and some inclusions (black). Now we will run simulation with some parameters for example HexRandom neighborhood Rule1-4 and periodic boundary condition

Tools

New Grain Grain to save save

Andrzej Add Energy go all Test

Energy for Grain

☒ Energy Homogenous in grain  
☐ Energy Heterogenous  
☐ Energy Homogenous

☒ Structure ☒ 1 ☐ -  
☐ Energy ☐ + ☐ =

☒ Periodic Boundary Conditions  
☐ Absorbing Boundary Conditions

☐ Von Neumann ☐ Rule1  
☐ Moor ☒ Rule1-4  
☒ Hex Random ☐ Montecarlo  
☐ Penta Random  
☐ Hex\ 1  
☐ Hex/  
☐ Further Moor Change

Size of Dislocation Number of Grains

Circle random add Square

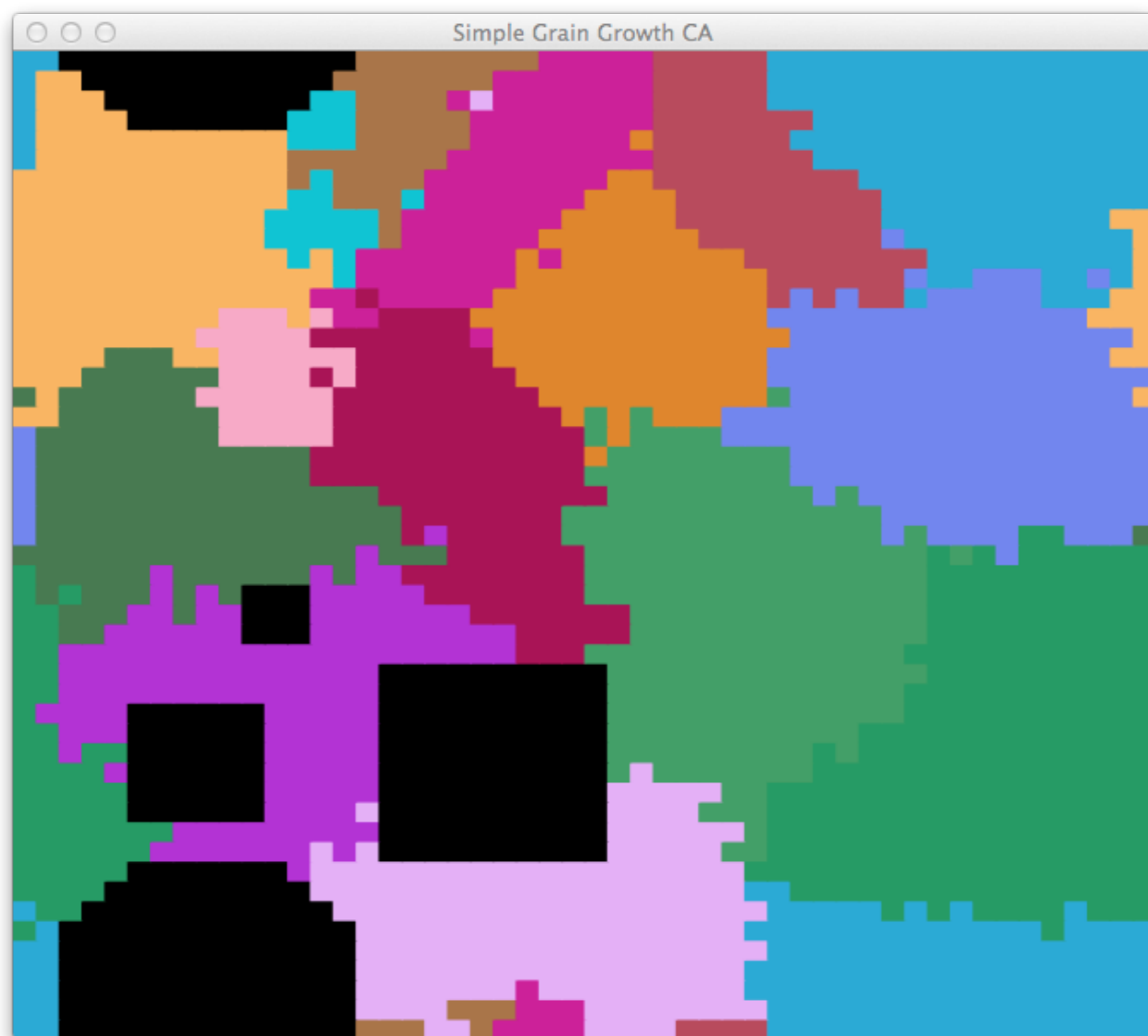
Clean random add grains zej To End

Info:

Here we can see (I will describe only elements relevant to this project):

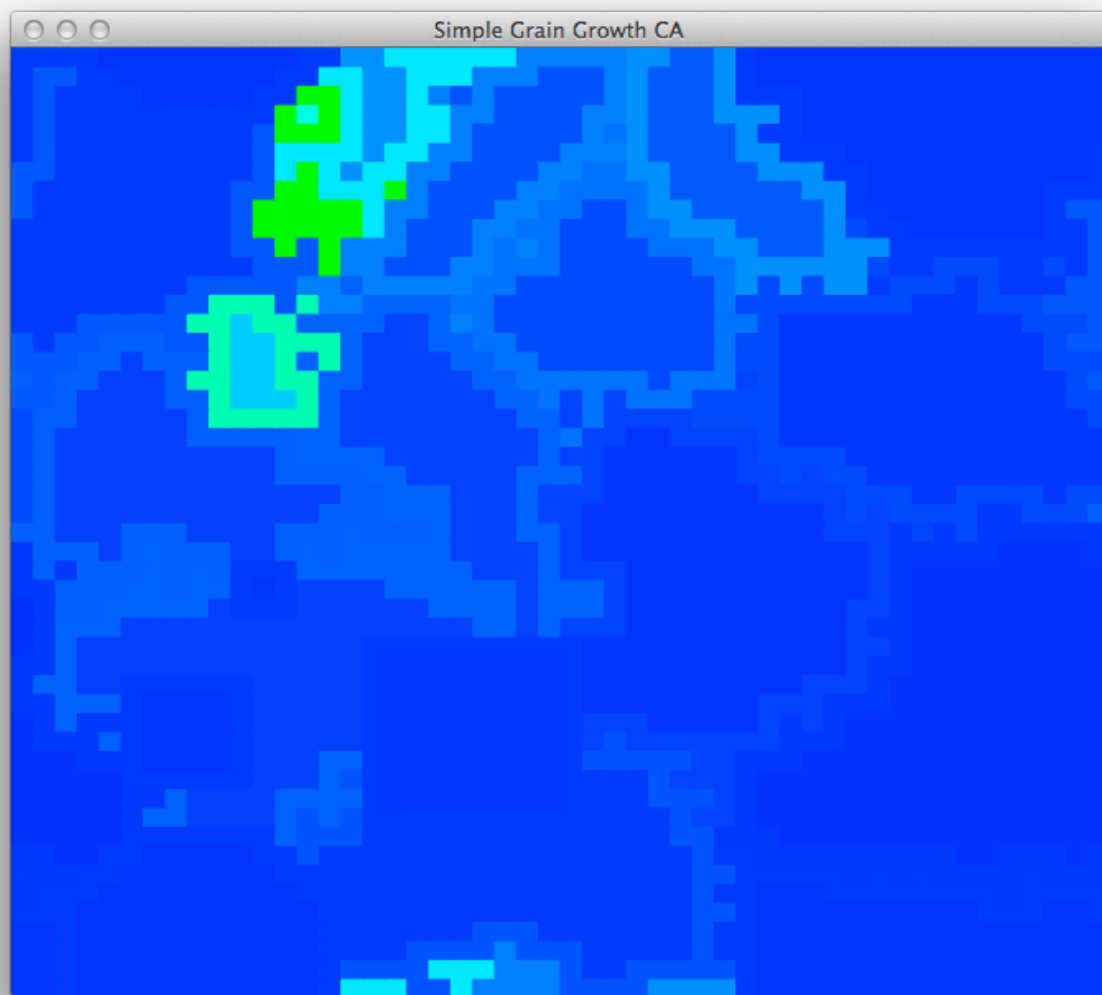
button to add energy to grains  
button to execute one iteration  
text field with amount of energy to add  
choose energy distribution  
choose display type  
choose nucleation rules  
add some random grains

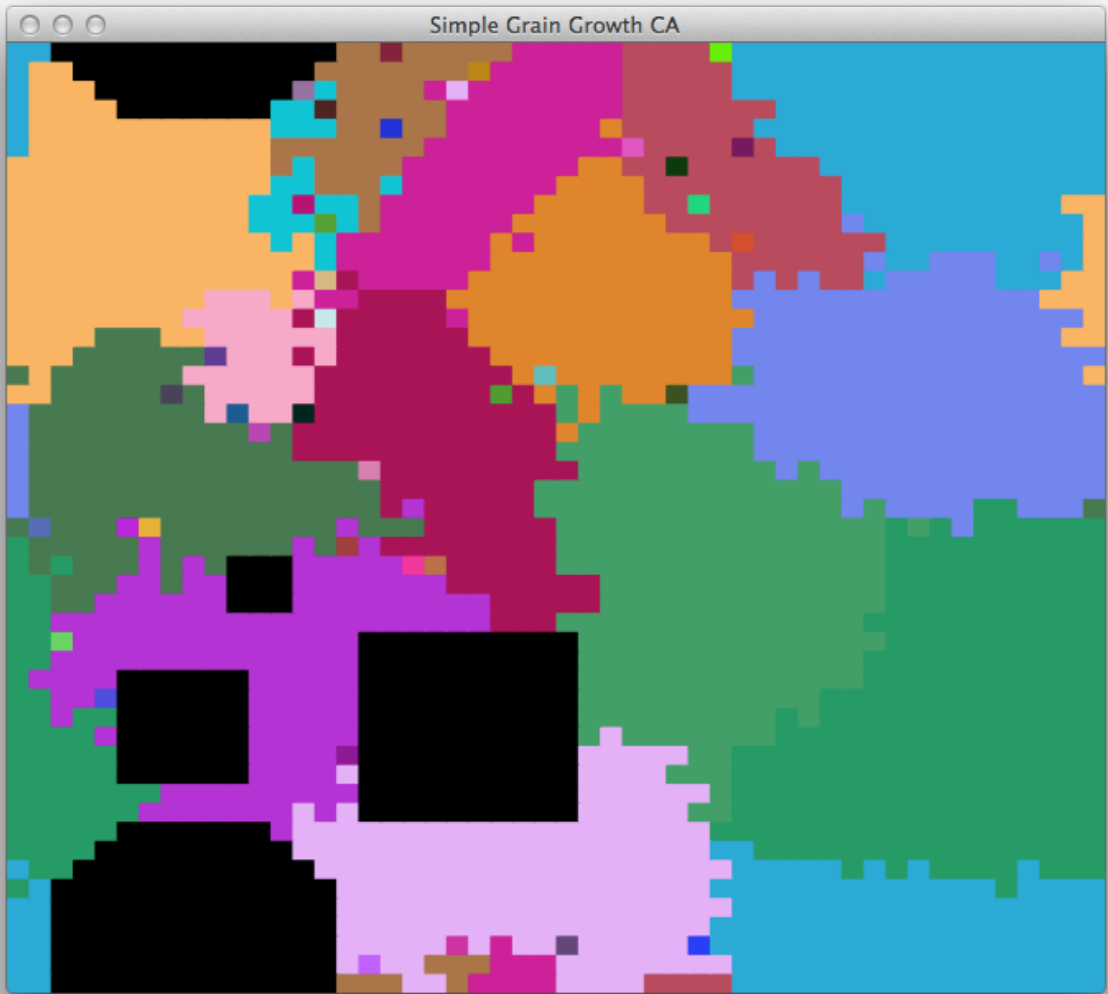
now we can generate structure



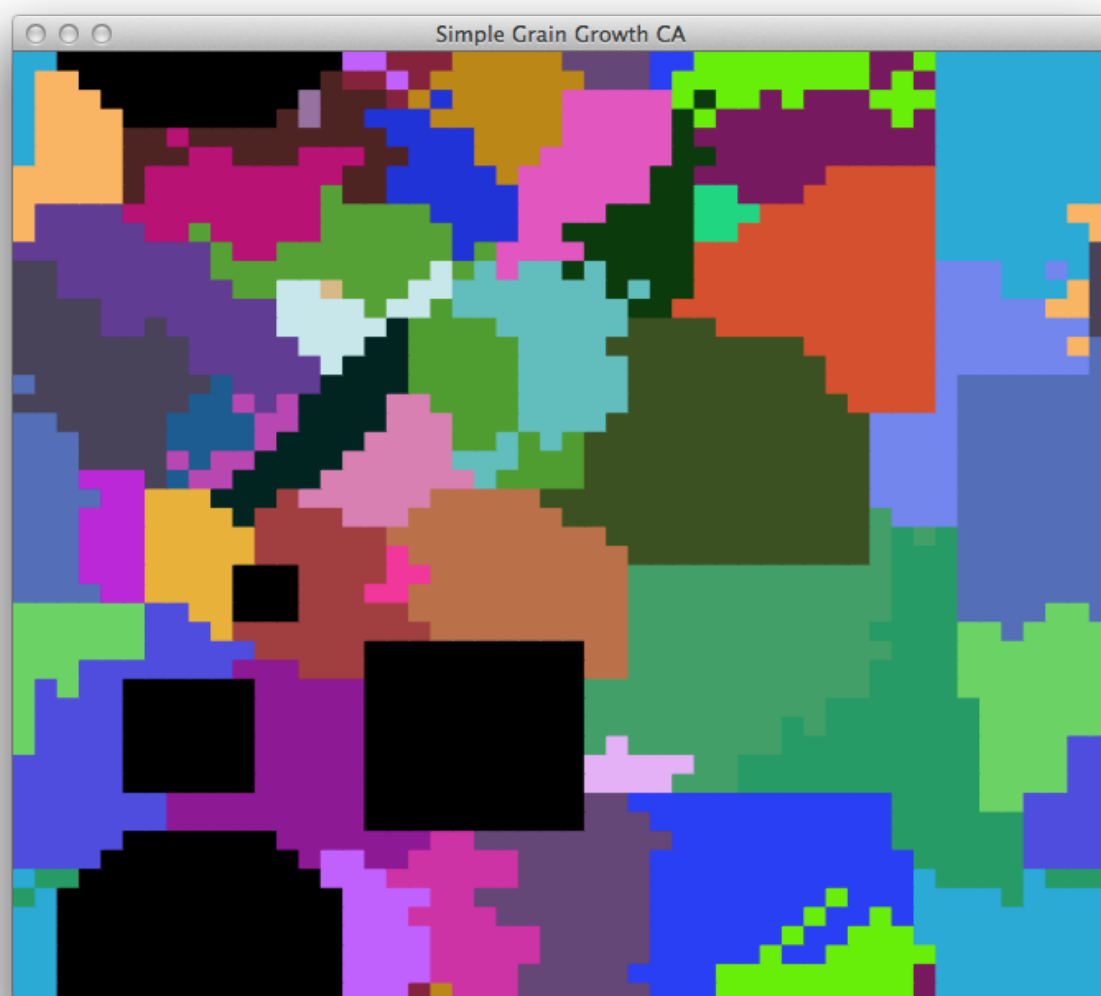


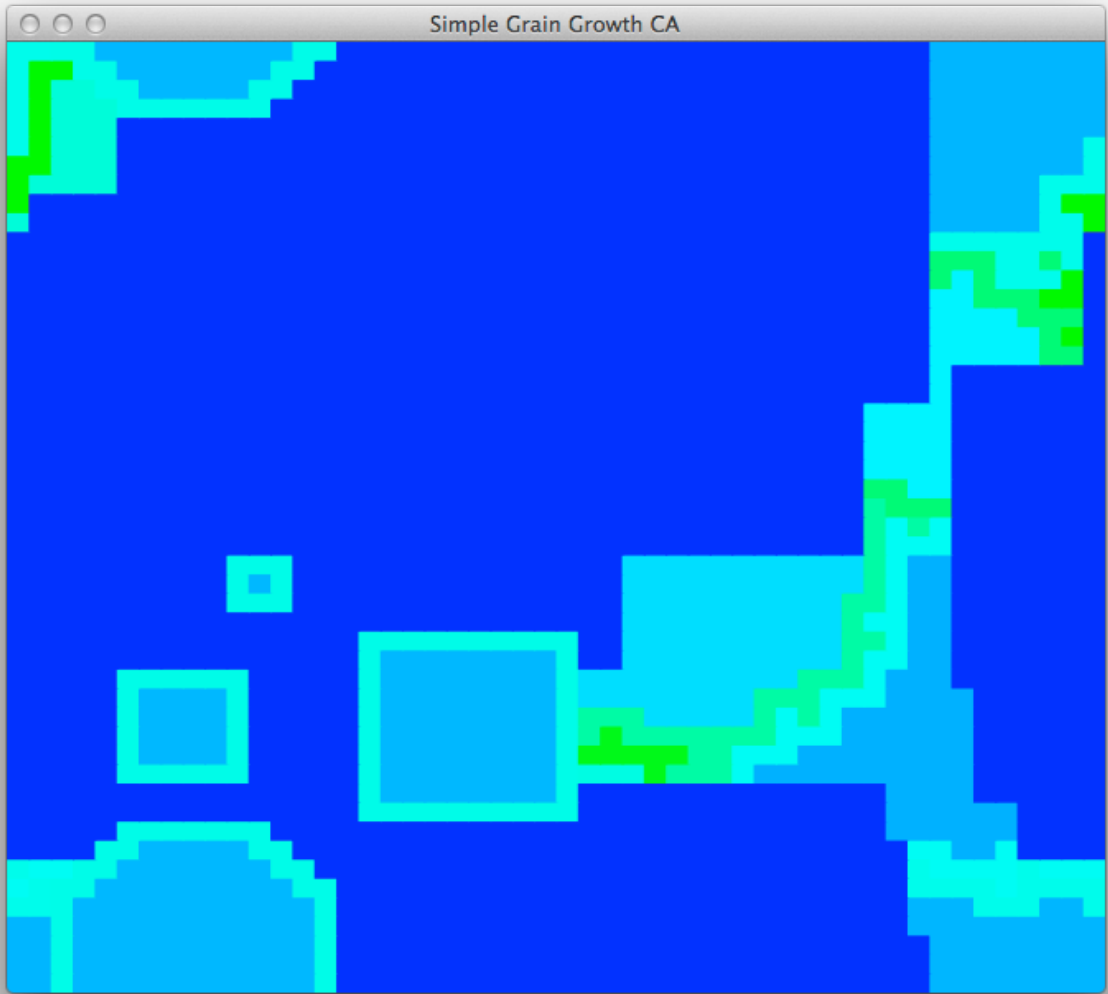
lets add some energy



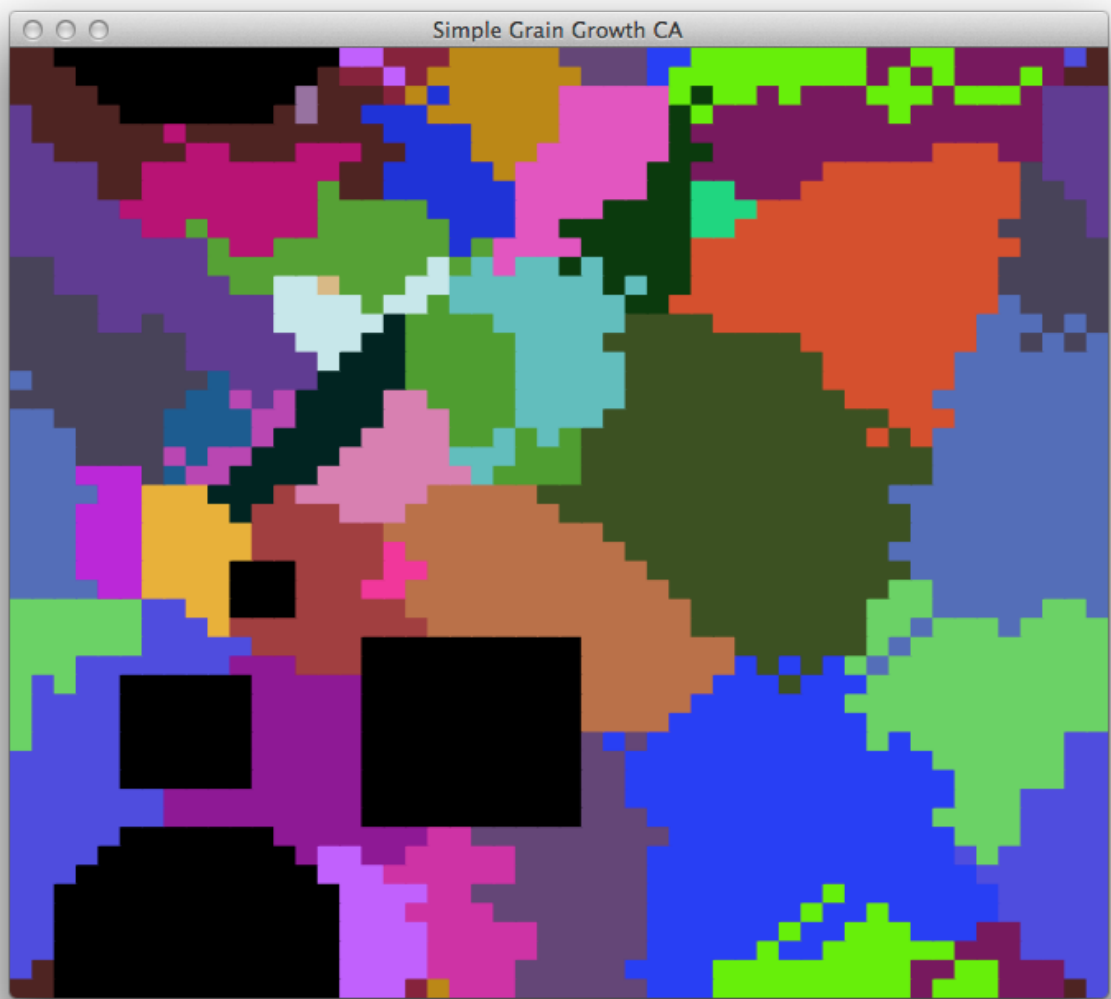


now we can growth them with Montecarlo





energy view



## Time comparison

Grain Growth + SRX Time

	Time in seconds	Time per Cell in seconds
Moore	842	0.000585
Numan	635	0.000441
Penta	674	0.000468
My Code (Moore)	10	0.001000

As you can see my code is very slow.

My code was operating on 100x100 space. The grid code was operating on 1200x1200x1 space.

# Conclusions

My conclusions after writing this code & testing MCMicro

- Monte Carlo method is quite interesting and with stochastic behavior
- My code has high requirements but it has not been optimized
- I can see some places when we can use GPU in my code
- My code should be fairly easy to parallelize
- My code is very slow compared to the grid
- It would be very useful to have the config file in xml format