

SPPARKS

```
#include "string.h"
#include "spparks.h"
#include "memory.h"
#include "error.h"
#include "universe.h"
#include "input.h"
#include "output.h"
```

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SPPARKS for microstructural science

Brian DeCost

```
#include "potential.h"
#include "random_mars.h"
#include "timer.h"
#include "output.h"
```

```
using namespace SPPARKS_NS;
```

```
/* ----- 11 July 2014 -----
   allocate fundamental classes (memory, error, universe, input)
   parse input switches
   initialize communicators, screen & logfile output
   input is allocated at end after MPI info is setup
   ----- */
```

```
SPPARKS::SPPARKS(int nargs, char **arg, MPI_Comm communicator)
{
    error = new Error(this);
```

Stochastic Parallel PARticle Kinetic Simulator¹

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SPPARKS is an efficient *parallel* Kinetic Monte Carlo framework

- ▷ Mesoscale materials phenomena as stochastic processes
- ▷ Scalable to thousands of processors
- ▷ Modular C++ facilitates user-defined models/statistics
- ▷ Open Source (GPLv2)
- ▷ Related to the LAMMPS Molecular Dynamics framework

¹<http://spparks.sandia.gov/>

How SPPARKS is used

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SPPARKS is a command-line application. Simulations are defined by input scripts composed of **SPPARKS commands**

The most important commands are:

- ▷ `app_style`
- ▷ `solve_style` / `sweep_style`
- ▷ `diag_style`

What applications is SPPARKS useful for?

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- ▷ lattice-based models
- ▷ off-lattice models
- ▷ generic KMC applications

In this session, we'll focus on the Potts model

- ▷ Modeling grain growth, recrystallization, and related phenomena
- ▷ Annealing synthetic microstructures to achieve local equilibrium along triple lines
- ▷ Generation of simple synthetic microstructures

The SPPARKS distribution

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Download **SPPARKS** from

<http://www.sandia.gov/~sjplimp/download.html>

Unpack the SPPARKS source archive

```
mkdir -p ~/Software && cd ~/Software  
tar xvzf ~/Downloads/spparks.tar.gz  
cd spparks*/src  
ls ~/Software/spparks*/
```

```
brian@eeepc:spparks-19Nov13 $ ls ~/Software/spparks-19Nov13  
doc  examples  LICENSE  python  README  src  tools
```

SPPARKS uses the Unix build system make

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SPPARKS is distributed with several makefiles, found in `src/MAKE/`.

```
bdecost@unix6 > ls MAKE ~/Software/spparks-19Nov13/src
Makefile.blackrose  Makefile.mac        Makefile.serial
Makefile.cygwin     Makefile.mac_debug  Makefile.serial_backup
Makefile.g++        Makefile.mac_mpi    Makefile.serial_debug
Makefile.linux      Makefile.redsky     Makefile.xt5
```

You will likely have to edit `Makefile.linux`, `Makefile.g++`, or `Makefile.mac_mpi` to reflect your system to get SPPARKS to compile.²

²You'll likely need to supply the location of the MPI library files on your system.

Building SPPARKS

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Try to compile SPPARKS by running make with the appropriate build target for your system as an argument.

Building SPPARKS using Makefile.mac_mpi

```
make -j4 mac_mpi
```

The result is an executable named `spk_mac_mpi` in `src/`.

Building serial SPPARKS

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The JPEG library can also cause build problems which are difficult to resolve. Makefile.demo will build a serial version of SPPARKS without the JPEG library.

First build the MPI stubs:

```
cd STUBS  
make  
cd ..
```

Copy Makefile.demo into src/MAKE/

Build the demo version of SPPARKS

```
make demo
```


“Installing” SPPARKS³

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To avoid copying the SPPARKS executable or typing the full path to it repeatedly, define a *shell alias*:

```
alias spk='~/Software/spparks*/src/spk_demo'
```

Now typing `spk` into the shell prompt from any working directory runs SPPARKS. Try this now.

³To make this persistent, append this command to `~/.bashrc` (`~/.bash_profile` on a mac)

Running SPPARKS with no input

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SPPARKS reads commands from stdin

```
brian@rsfern > spk  
SPPARKS (19 Nov 2013)
```



Press Ctrl-C to exit.

Demo: SPPARKS input scripts

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SPPARKS is controlled by a script of commands which are executed line-by-line.

Run the basic demo

```
cd ~/Downloads/spparks-demo-master/demos/basic  
spk < basic.spkin
```

SPPARKS will print some diagnostic information to the screen, and to a log file called `log.spparks`.

SPPARKS output

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```
brian@rsfern > spk < basic.spkin
SPPARKS (19 Nov 2013)
Created box = (0 0 0) to (32 32 32)
  1 by 1 by 1 processor grid
Creating sites ...
```

```
  32768 sites
  32768 sites have 26 neighbors
Setting site values ...
  32768 settings made for site
Setting up run ...
```

	Time	Naccept	Nreject	Nsweeps	CPU	Energy
	0	0	0	0	0	843324
Demo:	10.0008	166567	0	0	6.46	301516
SPPARKS	20.0003	187372	0	0	6.93	243102
input scripts	30.0003	201713	0	0	7.19	206800
Demo: Grain	40.0001	213353	0	0	7.39	179268
growth	50.0001	222915	0	0	7.58	159700
kinetics	60.0033	231650	0	0	7.74	141190
Demo:	70.0009	238089	0	0	7.85	130340
Visualization	80.0003	243626	0	0	7.95	124082
with	90.0005	248183	0	0	8.02	119936
ParaView	100	252342	0	0	8.09	116864

```
Loop time of 8.09225 on 1 procs
```

```
Solve time (%) = 0.133569 (1.65058)
Update time (%) = 0 (0)
Comm time (%) = 0 (0)
Outpt time (%) = 0.0541012 (0.668556)
App time (%) = 7.87678 (97.3373)
Other time (%) = 0.0278049 (0.343599)
```

Anatomy of an input script: basic.spkin

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```
# Minimal SPPARKS Potts script
seed                56789
app_style            potts 100
dimension            3
lattice              sc/26n 1.0
region               box block 0 32 0 32 0 32
create_box           box
create_sites         box
set                  site range 1 100
solve_style          tree
temperature          0.0
diag_style           energy
stats                10.0
run                  100.0
```

Demo: Grain growth kinetics

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Run the grain-growth-kinetics demo

```
cd ../grain-growth-kinetics  
spk < potts2d.spkin
```

This script uses the cluster diagnostic, which computes grain size information.

Grain growth kinetics

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This demo includes a python script which extracts grain growth kinetics from `log.spparks` and attempts to plot them.

Run the python script

```
python parse_log.py log.spparks
```

The script produces a file `cluster-stats.csv` that you can open in Excel.

Grain growth kinetics

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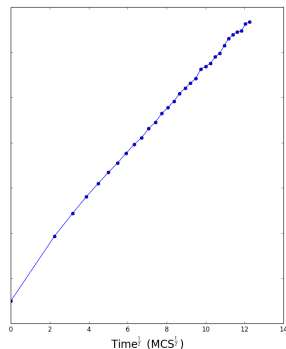
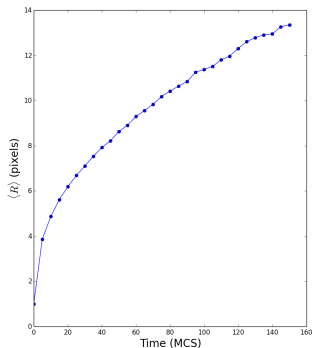
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Grain size is linear in sqrt-time!



The dump command

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Post-processing. `pizza.py` or custom scripts.

Conversion to vtk with pizza.py

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The python script `pizza_dump2vtk.py` uses tools from the open source [pizza.py](#) toolkit to create vtk files from the SPPARKS many-timestep dump file.

Run `pizza_dump2vtk.py`

```
python pizza_dump2vtk.py potts.dump
```

Visualizing with ParaView

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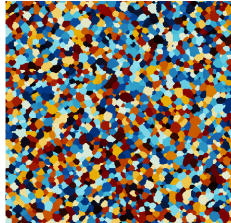
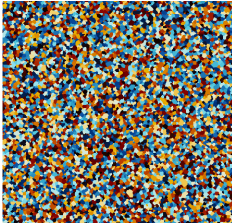
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Open the vtk files in ParaView to create a movie.



mpirun

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Processor partitions

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