

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 Simulator<sup>1</sup>

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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

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<sup>1</sup><http://spparks.sandia.gov/>

# 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.<sup>2</sup>

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<sup>2</sup>You'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” SPPARKS<sup>3</sup>

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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.

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<sup>3</sup>To 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

## SPPARKS

```
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

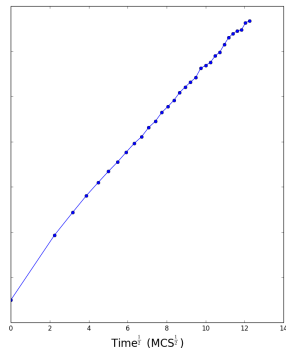
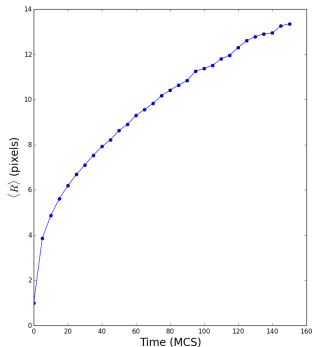
```
python parse_log.py log.spparks
```

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

# Grain growth kinetics

## SPPARKS

Grain size is linear in sqrt-time!



# The dump command

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



# Installing pizza.py<sup>4</sup>

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Download and unpack the pizza.py archive from  
<http://www.sandia.gov/~sjplimp/download.html>

### Unpack the SPPARKS source archive

```
mkdir -p ~/Software && cd ~/Software  
tar xvzf ~/Downloads/pizza.tar.gz  
cd -  
alias pizza='python -i ~/Software/pizza*/src/pizza.py'
```

---

<sup>4</sup>As with SPPARKS, append the alias command to ~/.bashrc or  
~/.bash\_profile to make this “installation” persistent.

# Conversion to vtk with pizza.py

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# Visualizing grain growth

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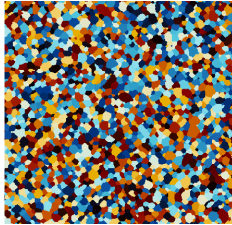
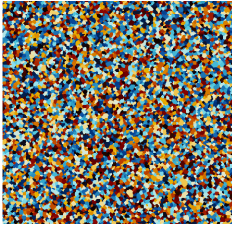
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# mpirun

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# Processor partitions

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