

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 **PAR**ticle 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 (GPLv3)
- ▷ Related to the LAMMPS Molecular Dynamics framework

¹<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

Spatially decomposed parallelization

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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.

A basic 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
diag_style           energy
stats                10.0
run                  100.0
```

Diagnostics

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Log file

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The dump command

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

Installing pizza.py⁴

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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'
```

⁴As 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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mpirun

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Processor partitions

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