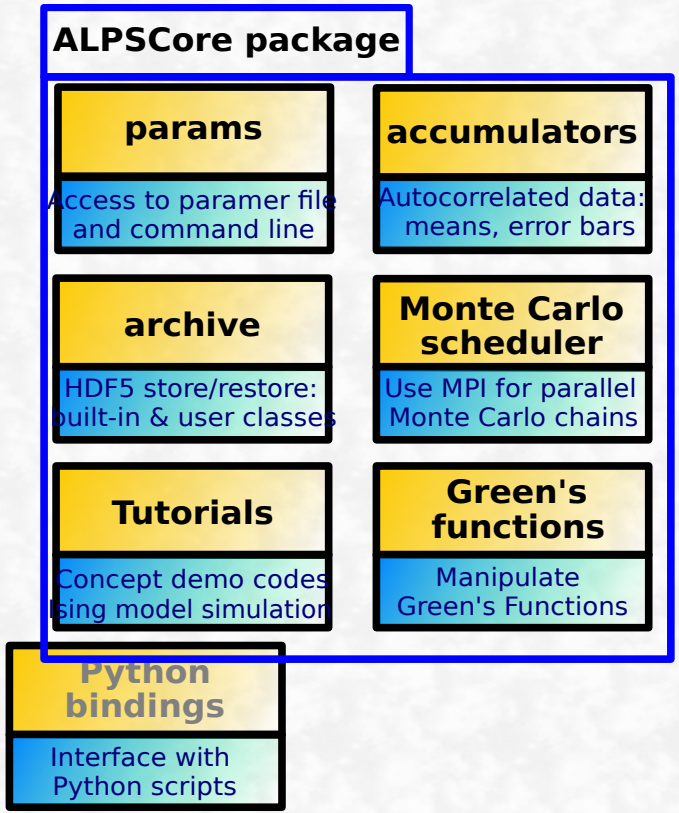
What is ALPSCore?

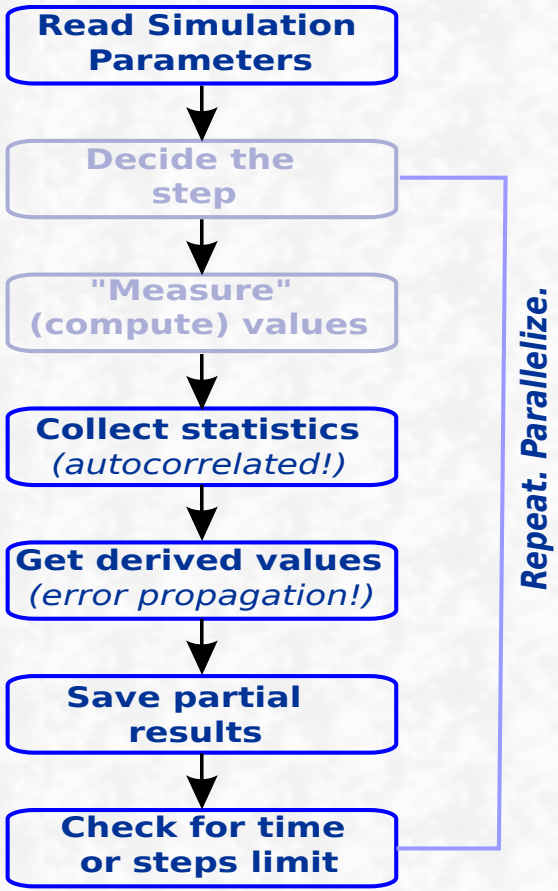
- Software library for writing physics simulation codes
- Primarily for Monte Carlo methods (as of now).

However...

- Has support for Green's Functions;
- Support for lattices is planned.



Why use ALPSCore?



Look at a typical simulation:

- A lot of „boilerplate“ code;
- Often non-trivial;
- Performance is important!
- Python (or other scripting): hard to combine with C++

ALPSCore helps to focus on science!

Brief history of ALPSCore

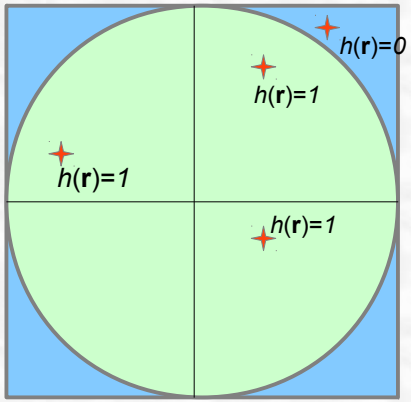
- ALPSCore is the "core ALPS library"
- ALPS is "Algorithms and Libraries for Physics Simulations" (see http://alps.comp-phys.org)
- ALPSCore goals:
  - Be more compact
  - Faster development cycle
  - More extensive documentation.
- Focuses on the most often used components.

What is the plan for this tutorial?

1. Assume that ALPSCore is installed!
2. Make a very simple Monte Carlo simulation demo.
3. Parallelize the demo.
4. Make a 2D Ising model simulaton code.

Exercise 1: Preface

Task: Compute π by Monte Carlo method.



$$\frac{S_{cir}}{S_{sqr}} = \frac{\pi}{4}$$

"hit function" $h(\boldsymbol{r}) = \begin{cases} 1 \text{ for } \boldsymbol{r} \in \text{Cir} \\ 0 \text{ for } \boldsymbol{r} \notin \text{Cir} \end{cases}$

$$\frac{S_{cir}}{S_{sqr}} = \frac{N_{cir}}{N_{sqr}} = \frac{1}{N}\sum_{i=1}^{N} h(\boldsymbol{r}_i) = \langle h \rangle$$

It is not hard to write the program to compute the mean <h>.
But...

What about error bars?
Do you really remember those formulas? 🙂

Exercise 1: Implementation specifics

Directory: `step1_pi/`

`CMakeLists.txt` specifies application structure

`simulation.hpp` describes simulation class (the model)

`constructor:` constructs the model

`update():` performs MC trial *`measure():`* measures the quantities

`fraction_completed():` are we done yet?

`simulation.cpp` implements the model

`main.cpp` sets up and runs the simulation

Let's look at the code!

Exercise 1: Implementation specifics

`simulation.cpp` `main.cpp`

Code uses *parameters* : to allow user to pass input data

Each parameter has:

- ✔ Name (*e.g.* `"trials"`)
- ✔ Type (*e.g.* `int`)
- ✔ Description (*e.g.* `"Number of trials"`)
- ✔ Optionally: a *default value*

`define_parameters()` is responsible for defining simulation-specific parameters

Let's look at the code!

Exercise 1: Hands-on

Task: Computing π by Monte Carlo method.

1. Build the program:

```
$ mkdir 000build
$ cd 000build
$ cmake ..
$ make
```

2. Run without arguments:

```
$ ./alpsdemo
```

3. Request help:

```
$ ./alpsdemo --help
```

4. Timed runs, varying trial count:

```
$ time -p ./alpsdemo --trials=100
```

5. Timed runs, varying time limits:

```
$ time -p ./alpsdemo \
   --trials=999999 \
   --timelimit=10
```

6. Start a long run; then press **Ctrl-C**; observe graceful termination.

Exercise 1: Hands-on, continued

Task: Use parameter file; play with the code.

7. Use parameter file:

```
$ ./alpsdemo ../demo.ini
```

8. Override params from file:

```
$ ./alpsdemo ../demo.ini \
    --trials=9999
```

9. Change the code: make `--trials=0` mean "till timeout"

File "demo.ini" :

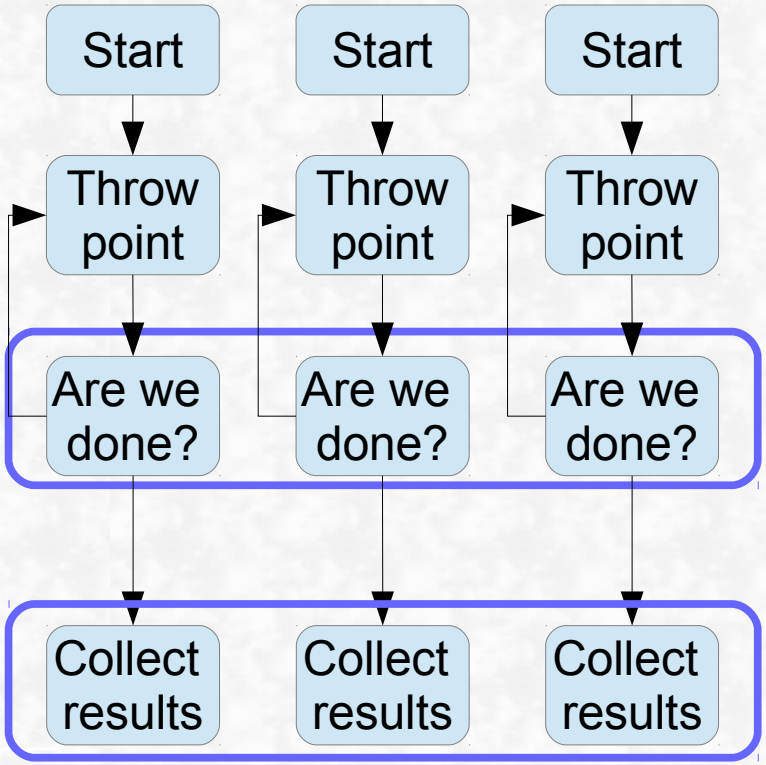
```
# how long to run?
timelimit = 100

# how many trials?
trials = 1000
```

Exercise 1: Take-home message

1. Linking `ALPSCore` to your application is very simple.
2. Most of the framework is ready-made for you; you only code "science";
3. You get parameters, scheduling, graceful termination, and error bars — all provided by the library.

Exercise 2: Preface

Point throwing can be done independently!



- Completion check requires occasional communications;
- Results are collected from all processes;
- The rest is completely parallel!

Exercise 2: Hands-on

Task: Compute π in parallel.

1. Examine the differences (main`.diff`):
   1. An adapter class is used.
   2. MPI is initialized.
   3. A few operations are parallel-aware.
   4. Only master process should print.

Let's look at the code!

Directory:
`step2_parallel_pi/`

2. Build and run the program:

```
$ mkdir 000build
$ cd 000build
$ cmake ..
$ make
$ ./alpsdemo --help
```

3. Do timed runs:

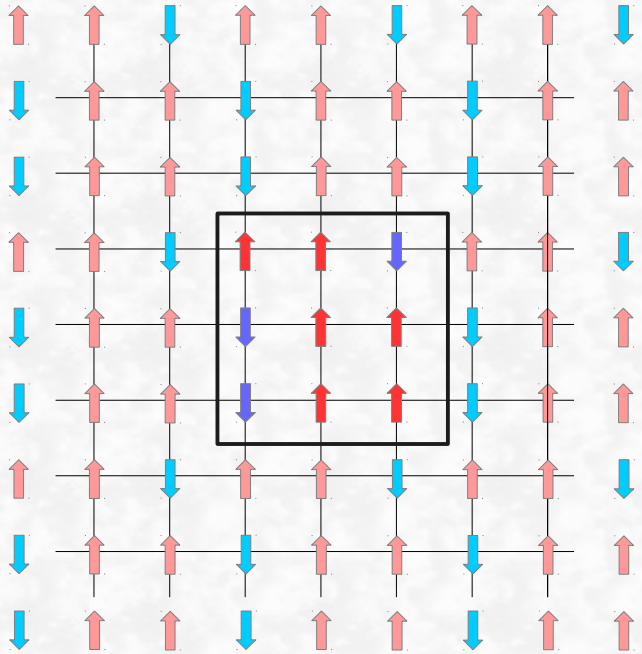
```
$ time -p mpiexec -n 1 \
    ./alpsdemo --trials=999999

$ time -p mpiexec -n 2 \
    ./alpsdemo --trials=999999
```

Exercise 2: Take-home message

1. Once you implemented serial MC,
   it's easy to make it parallel.
2. The requested MC steps are distributed
   among the parallel processes.
3. The processes occasionally communicate,
   to check if it's time to stop.

Exercise 3: Preface

Task: "Physics" problem: 2D Ising model.



Energy: $$E = -\frac{1}{N}\sum_{(i,j)} s_i s_j$$

Magnetization: $$M = \frac{1}{N}\sum_{i} s_i$$

Temperature *T*

Mean values: $$\langle E\rangle, \langle M\rangle, \langle |M| \rangle, \langle M^2\rangle, \langle M^4\rangle$$

Binder Cumulant: $$U = 1 - \frac{\langle M^4\rangle}{3\langle M^2\rangle^2}$$

Exercise 3: Approach

Task: "Physics" problem: 2D Ising model.

Monte Carlo step:

1. Flip a random spin;
2. Update energy;
3. Update magnetization;
4. Accept or reject update.

Problem: Measurements are *correlated*.

1. Naive approach: too narrow error bars;
2. Use `LogBinningAccumulator` for the correlated data;
3. Use `FullBinning Accumulator` if you need arithmetic.

Let's look at the code!

Exercise 3: Hands-on

Task: Try different simulation parameters and accumulators.

1. Build and run the code

2. Use parameter file with different accumulators:

```
$ ./ising2_mc  ../ising.ini  --acc=fullbin
$ ./ising2_mc  ../ising.ini  --acc=nobin
$ ./ising2_mc  ../ising.ini  --acc=logbin
```

Note different error bars.

3. Extra points: parallelize the code!
   1) Use `mcmpiadapter` class template;
   2) Initialize MPI environment;
   3) Pass the communicator to params and simulation constructors;
   4) Make sure only master prints.