

ALPSCore Tutorial

DRAFT Version 2

Alexander Gaenko
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ALPSCore tutorial: links

These slides:

<https://git.io/alpscore-tut-2017-02-24>

Accompanying code:

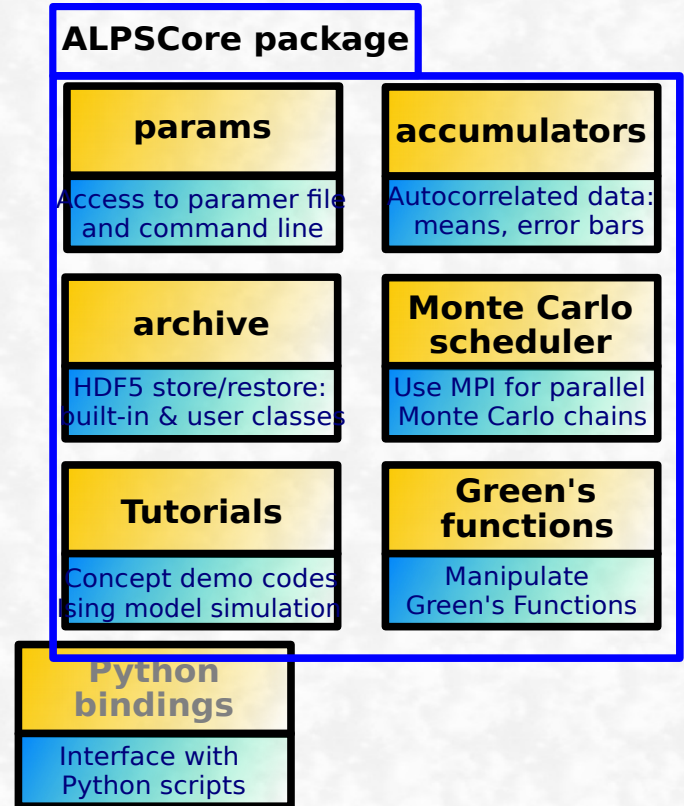
https://github.com/galexv/ALPSCore_Tutorial2

What is ALPSCore?

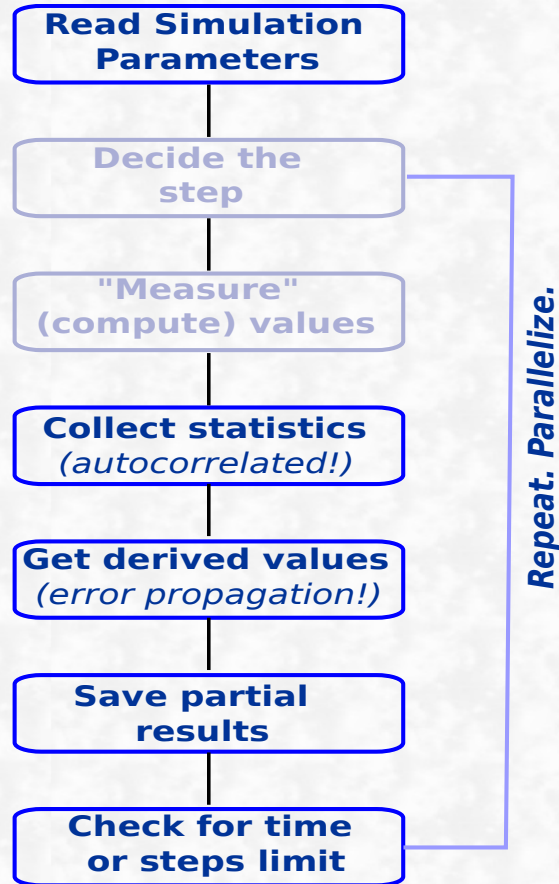
- Software library for writing physics simulation codes
- Primarily for Monte Carlo methods (as of now).

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

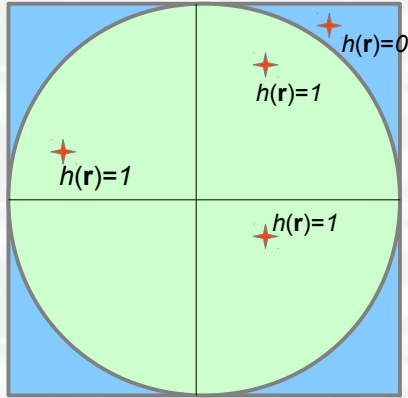
- ALPSCore is the "core ALPS library"
- ALPS is "Algorithms and Libraries for Physics Simulations" (see <http://alps.comp-phys.org>)
- ALPSCore goals:
 - ✓ Be more compact
 - ✓ Faster development cycle
 - ✓ More extensive documentation.
- Focuses on the most often used components.

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 simulation code.

Exercise 1: Preface

Task: Compute π by Monte Carlo method.



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

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

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

It is not hard to write the program to compute the mean $\langle h \rangle$.

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)

[simulation.cpp](#)

implements the model

constructor: constructs the model

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

fraction_completed(): are we done yet?

[main.cpp](#)

sets up and runs the simulation

Let's look at the code!

([orange](#) and [blue](#)
are clickable – try!)

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!

(remember,
orange and **blue**
are clickable!)

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"
(*solution*)

File "*demo.ini*" :

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

```
# how many trials?  
trials = 1000
```

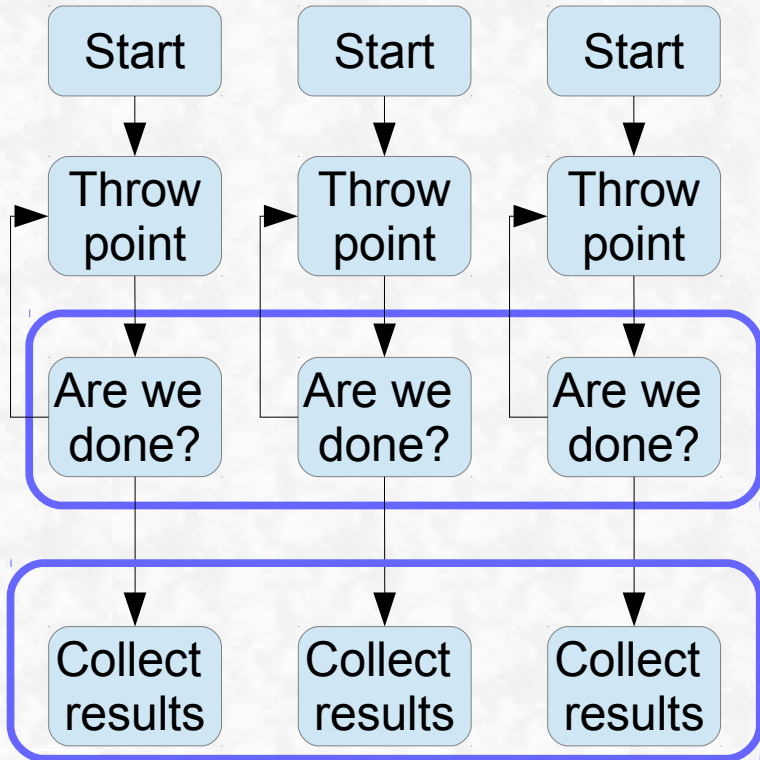
(remember,
orange is clickable!)

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.

Let's look at the code!

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

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

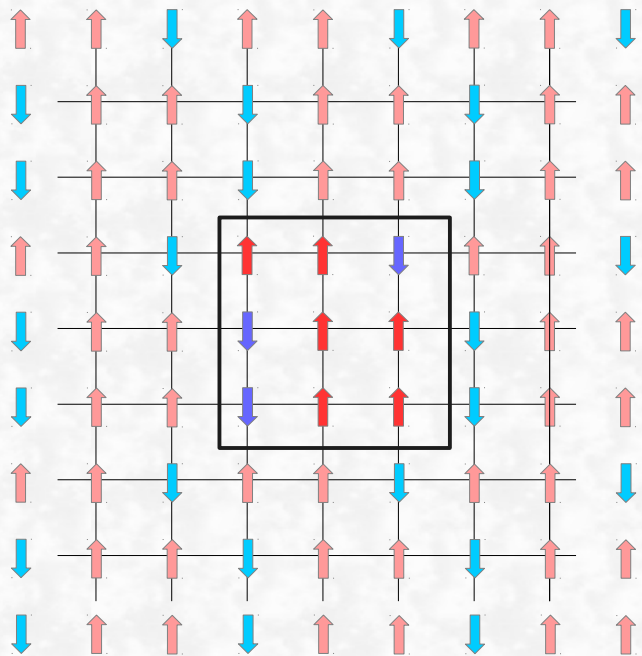
$ time -p mpiexec -n 2 \
    ./alpsdemo --trials=999999
```

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 ;
$$\beta = 1/T$$

Boltzmann distribution:
$$p_i \sim e^{-\beta E}$$

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.

Directory: `step3_ising/`

Monte Carlo step:

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

Let's look at the code!

Problem: Measurements are *correlated*.

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

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
```

Look at energy and Binder Cumulant.
Note different error bars!

3. Extra points: parallelize!

1) Use mcmpiadapter

2) Initialize MPI

3) Pass communicator to:
params
simulation constructors

4) Make sure only
master prints.

Exercise 3: Take-home message

1. ALPSCore provides means to collect statistics properly;
2. Autocorrelation results in too optimistic error bars;
3. Use binning accumulators (preferably FullBinning) for your Markov chain simulations.