

# Thesis Notes

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## Monday, June 15

- Preliminary meeting
- We will begin with  $\phi^4$  term due to lower energy bound.
- Beginning with code in Python, switch to C/C++ if necessary.

## Tuesday, June 16

- Preliminary concepts to understand:
  - scalar field theory on lattice
  - Markov chains and Monte Carlo
  - the gradient flow
  - $O(n)$  symmetry
- General components to research, executed in parallel
  - Reading
  - Mathematical analysis
  - Writing code
  - Present (writing, plot generation,...)
- Things to get out of dissertation (Schaich and Loinaz 2006)
  - Markov chain
  - Cluster algorithms
    - \* Metropolis is a method for narrowing possibilities by accepting only some changes. It can get stuck in a local minimum, loss of ergodicity. We solve these with cluster algorithms. Wolff grows clus-

ters probabilistically and flips, while Swenson and Yang identifies clusters and flips them probabilistically.

- \* Near a phase transition, correlation length grows and changes become less likely to be accepted: need clusters. Clusters don't work far from the phase transition. This is manifested as a sequence of a few metropolis steps and a cluster step.

- Research plan

- Start with 2D  $\phi^4$ 
  - \* Set up lattice with sign flip for reflection
  - \* Use Markov chain Monte Carlo to simulate.
  - \* Measure, magnetization and susceptibility, Binder cumulant
- Transition to 3D, then maybe transition to C/C++.
- Implement the gradient flow
- move to 2-3d nonlinear sigma model.
- Motivation: the nonlinear sigma model works for QCD given the asymptotic freedom. We may also want to explore topology.

## Wednesday, June 17

- Code tips:
  - Try Swendsen-Wang algorithm in addition to Wolff
  - Print out time taken
  - Optimize Hamiltonian
  - Save every tenth measurement or store configurations to calculate path integral. Exclude thermalization (first 200)
  - Write in terms of sweeps, not iterations
  - Parallelize (look into checkerboard algorithm)
  - Implement Binder cumulant and susceptibility
  - Store every few states
  - Look into multigrid algorithm
- Reading on Monte Carlo Markov chain and cluster algorithms.

## Friday, June 19

- Looking over code
  - Might be too slow, move to C/C++ eventually?
  - Why is the energy increasing with metropolis algorithm?
  - Shift to using action instead of Hamiltonian.
  - Transition from Broken Phase, look at  $\mu_0^2$  term.
  - Profile code for possible optimizations.

## Monday, June 22

- Coding
  - Add plots to `.gitignore`.
  - Try parallelizing code, using either multigrid or checkerboard algorithm
- Reading
  - Start to focus more on understanding the theory behind research.
  - Read dissertation (Schaich and Loinaz 2006) Chap. 6.5 and 6.6, take notes on questions.
  - Newman (Newman and Barkema 1999) (Main textbook for Monte Carlo in Statistical Physics)
- Just some things to remember
  - Correlation functions correlate values in statistical systems and relate to propagators in QFT.
  - The problem of renormalization:  $a \rightarrow 0$  leads to unbounded correlation function. As real physical lengths are measured in terms of the lattice constant, these sometimes tend to infinity.

## Wednesday, June 24

- Code
  - Parallelize
  - Transition to numpy
- Theory Question
  - renormalize and regularize: what do they mean?
  - Look at LePage

## Tuesday, June 30

- Code
  - Try `mpi4py`.
  - Move to 3D (this may decrease parallel overhead)
- Reading
  - Continue Reading Collins, others.

## Thursday, July 2

- Coding
  - Continue implementing MPI
  - Parallelization may be more apparent in 3D
- Reading
  - Dirac fermions, represented by 4D spinor field (spin up/down, electron/positron)
  - Look at Tong (Chap. 4)
  - Charge (See Tong, Noether's Theorem)
- Next week back: start gradient flow on linear  $\phi^4$  model

## Monday, July 13

- Update from last week
  - Implemented MPI, slowdown may be due to thermal throttling?
  - Questions:
    - \* Noether's Theorem, 4-current?
    - \* Star vs. dagger
- Invariance vs covariance
  - $Q$  (charge) is invariant, not covariant. Derivative is 0 (conserved) so no effect of boost. See (StackExchange)[<https://physics.stackexchange.com/questions/270296/what-is-the-difference-between-lorentz-invariant-and-lorentz-covariant>]
- Operator product expansion
  - Taylor (Laurent in reality) series for operators
  - Used to expand nonlocal (slightly) operators using local operators
- TODO:
  - Read conference proceedings, then paper with Orginos
  - Define  $\rho$  field (Eq. 2.4), implement it using the exact solution (Eq. 2.5). This will require a FFT

## Wednesday, July 15

- Code organization
  - Perhaps implement the nonlinear  $\sigma$  model (at a later date) and the  $\phi^4$  model as subclasses of a generic lattice class with abstract methods of action, etc.
- Gradient flow
  - Splitting momentum at half of lattice is a-ok.
  - Next, implement observable!
- New terms:
  - autocorrelation times (see Schaich -> MC Textbook -> Wolff): not a QFT concept!

- Gamma analysis: used to calculate autocorrelation
- summation window: part of the Gamma analysis
- Three classes of QFTs
  - renormalizable: infinities can be absorbed by a finite number of counterterms
  - nonrenormalizable: requires infinitely many counterterms
  - super-renormalizable: there is only one parameter that is divergent

## Friday, July 17

- Critical mass problem
  - Check multiple measures (Binder Cumulant, bimodality, etc.)
  - <https://journals.aps.org/prd/abstract/10.1103/PhysRevD.58.076003>
  - Infinite volume limit?
  - Turn off coupling?
  - Behavior for one node? Two nodes?
  - Metropolis checkerboard? (see (Schaich and Loinaz 2006, pg. 79))
  - Look at Schaich's calculations
  - Note: No true phase transition in finite system since phase transitions are defined by correlation lengths going to infinity

## Monday, July 20

- Remarks on critical point graph
  - I should be averaging the measurements from run.
  - Probably will need many more measurements.
  - Spend more time thermalizing
  - Calculate autocorrelation time, use to determine the `record_rate`
  - Production quality: try 10,000 sweeps, with 1000 thermalization
  - Run with slightly larger lattice to verify critical point
- Todo:

- Flow time dependence (with action)
- Average all measurements (incorporate this into `recorder.py`)
  - \* Plot mean and standard error as error bars
- Autocorrelation times using Gamma analysis
  - \* Paper has Mathematica notebook link, though it may be broken.
- Double check that large lattice volumes show correct critical mass.

## Wednesday, July 22

- Things I did:
  - Reorganized the `recorder.py` to include measurements and means/errors.
  -
- Questions:
  - Implementing the gradient flow: how does this play into the Monte Carlo simulation?
- TODO:
  - Critical mass
    - \* Plot histogram for two points of single lattice (thermalized)
    - \* See if this is affected by a large thermalization, cold start
    - \* Binder cumulant should be step function
  - Autocorrelation times
    - \* See Eq. 41
    - \* Get MatLab code
  - Gradient flow
    - \* Each measured lattice should be evolved in flow time before recording

## Friday, July 24

- Things to do:

- Gradient flow
- Try  $m_0^2 = -0.8$ , see if it become bimodal with large thermalization.
- Move towards critical value: does  $\tau_{int}$  increase? (This is what we expect)
- Perhaps change recording rate?
- Is it time to transcribe the code?
  - Explore efficiency boost
  - C++?
  - Cython?
  - Local cluster?

## Monday, July 27

- Shift to utilizing the 0th node for computation.
- Things to note:
  - Histogram in conference proceedings bins single lattice, not average over Markov chain.
- Questions:
  - collecting plots
- To-Do:
  - Run a proper histogram for different thermalizations, see if  $10^4$  is necessary.

## Wednesday, July 29

- Plots look good, but are a little wide and not localized on the convergent point
  - Try a cold start
  - Look at 256



- Average a couple trials
- To-Do:
  - See if I can find the width issue
  - Check autocorrelation times (with/without cluster)
    - \* close to critical value
  - wait on gradient flow until we are more confident in Markov chain.

## Friday, July 31

- Calculate autocorrelation times (as a function of mass), binder cumulant
- Check Wolff algorithm, try Swendsen Wang
- Multigrid algorithm?
- Focus on metropolis algorithm. We don't want to study a cluster algorithm on the backdrop of a broken metropolis algorithm.
- Literature search: must the metropolis algorithm have randomly included sites?

## Thursday, August 6

- Progress:
  - Autocorrelation: see page 6 from Schaich
    - \* Affected by the measurement rate?
  - Wolff implemented in C, large speed-up
  - Fixed neighbor bug in Wolff algorithm
  - Histogram issue still persists

## Friday, August 7

- Binder cumulant shows very different critical mass

- Going forward:
  - Start taking personal notes on the research with sketches, ideas, progress
  - Always calculate all of the observables
- Try the Binder Cumulant without Wolff
- See if the result depends on thermalization
  - This result should not be the same as 0 thermalization.

## Wednesday, August 12

- There are some major problems with my averaging.
- TODO: implement this fix

### Graduate School:

- Aim high
- Best possible school that you're happy at
- Name recognition matters
- If you can afford to do the applications, apply to a lot
- Maybe not scientific instrument lab?
- You will have a choice between famous advisors:
  - Famous: letters and papers will carry weight
  - Not-famous: much less attention
- Are you emailing your future advisor?
  - depends on place
  - At MIT, less important to single out a specific professor.
  - At a small school (W&M), you need to identify someone before hand.
    - \* People can actually change advisors

- Possible schools:

- UCSD
- Berkley
- Rutgers
- UMD
- UCSB
- MIT
- Yale

## Friday, August 14

- First, check previous version and make sure the numbers are not the same.
- Try saving some lattices, then calculating observables in Mathematica

## Tuesday, August 25

- Progress:
  - Fixed BC issue by fixing the order of calculations. New order:
    1. calculate volume-average
    2. take any exponents
    3. take the ensemble average
    4. compute any derived quantities
  - This is supported by Eq. 4.19 (Newman and Barkema 1999).
- Future work
  - Calculate errors for derived quantities using `gvar`.
  - Transition to GitHub (ID is `cjmonahan`).
  - Run through measurements that you can think of. Try other measurements (e.g. bimodality) and generate definitive list of plots.
  - Create plots without connected lines

## Thursday, August 27

- Problem with Binder-Cumulant: errors are too large.
  - Implement Jackknife method (see (Toussaint 1989)) to measure statistics of variables.
    - \* Try this on 128 lattice, maybe once overnight
  - Migrate to cluster
  - Or perhaps beforehand, try gradient flow.

## Tuesday, September 1

- Questions:
  - Do I apply it to every measurement?
    - \* Yes
  - Are flow time and Monte Carlo time independent?
    - \* Not really. This is actually where the gradient flow originates, but its not the point of our research.
  - What is the gradient flow scale?
    - \* We know that  $mass \times length$  is dimensionless, so we can measure the flow time in  $mass^{-1}$ .
    - \* In other more realistic theories, we can write the flow time as something physical, like the proton size.
    - \* In scalar field theory, we can do the same thing, but there is no physical analog.
    - \* The length scale of flow time should be written in terms of  $\lambda$  or  $m_0^2$ , with  $m_0^2$  being the slightly more natural choice.
- Todo:
  - Pick three fixed masses, study the flow time at each.
  - Evolve in flow time for each measurement.
  - Try this at  $N = 96$ .
  - Add the action as an observable.

## Friday, September 4

- Gradient flow should have a 0 imaginary component, so I can take the real component safely, though I should check this.
- Todo:
  - Add momentum constant to Gradient Flow evolution function.
  - Fix flow evolution bug!

## Tuesday, September 8

- Issue: Observable values are actually completely flat, may be a memory error in the code. This needs debugging.
- Plot the results on a smaller flow time scale.

## Friday, September 11

- Reminder: Must rescale momenta by  $\pi/L$ .
- Problem: Observables look flat
- We won't reproduce Figure 3 from proceedings.
- Continue to nonlinear sigma model.
  - Use (Aoki, Kikuchi, and Onogi 2015) to find other sources
  - Use inspirehep to find other sources.
  - Check out [[http://www.scholarpedia.org/article/Nonlinear\\_Sigma\\_model](http://www.scholarpedia.org/article/Nonlinear_Sigma_model)]

## Friday, September 18

- For Wolff algorithm, chose arbitrary vector to flip along.

## Tuesday, September 22

- Converting Cython to C++
  - Converting to flat lattice
  - Swendsen & Wang? we should implement this if Wolff works.
- The nonlinear  $\sigma$  lagrangian:
  - $g$  value is related to  $\sqrt{\lambda}$ .
  - also does affect system since factor of action is significant in path integral formalism.
  - No mass term.

## Friday, September 25

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- Questions:
  - New phi value, guarantee magnitude less than 1 with the other 3 components?
    - \* Should be using rotation matrices.
    - \* Take a look at SU(2) Metropolis literature and see how they generate norm-preserving rotation matrices computationally.
  - What exactly are we calculating?
    - \* Twist-2 operators
    - \* Condensates
      - VEV in non-perturbative theory.
    - \* Topology?
    - \* These could all be topics of our research
  - Prof. Chris: write notes next week about why the nonlinear  $\sigma$  model is “cool”.

## Wednesday, September 30

- Implement MPI in C++.
- There actually is an application of nonlinear-sigma, in fact multiple.
  - Heisenbuerg Ferro Magnetic, real application to condensed matter.
  - Applications to string theory.
  - Same properties as Yang-Mills Gauge Theories
    - \* O(2) renormalizable, nontopological solutions of classical EOM at finite action
    - \* Asymptotically free
    - \* Mass gap in nonperturbative theory
    - \* Large N limit
    - \* Dynamical generation of bosons, (like phonons, not explicit in Lagrangian).
  - In  $d = 4$ , the NLSM is starting point for chiral perturbation theory.

## Tuesday, October 6

- Added MPI to C++
  - Some issues with conversion to C array
- Make sure in implementation to keep lattice data continuous.

## Wednesday, October 14

- How to debug compilation errors?
  - Can't use print statements like Python.
  - I can use dummy routines to isolate issues.
- Priorities:
  - Ensure that Enrico's project is on the Arxiv while still doing work on my thesis in good faith.

## Wednesday, October 21

- Prof. Chris will ask Prof. Orginos about static memory allocation for rank and size.
- Code finally compiles!
- Action looks good but magnetization is incorrect.
  - Get other measurements (susceptibility, BC, etc.)
  - No need to export lattice average of  $\phi^2$ .

## Wednesday, October 28

- Progress
  - Plot with  $U$  and  $\chi$
  - I think I can statically allocate data in the Sweeper class using an initializer list.
- Do we need MPI?
  - Yes, in 3D it may be necessary since we won't have as many points.
  - Also is necessary for psychological help
  - Also allows adaptive sampling
- Mid Year report due Monday

## November 4

- Comparing Python and C++ part. Some issues:
  - Susceptibilities have errors that are too large.
  - Ratio of susceptibilities also wrong, expect a sharper dropoff.
  - Binder Cumulant has wrong final values, susceptibilities.
  - A good future solution is plotting the difference and a horizontal 0 line, also plot error.
  - I should rerun everything with the same data.
  - Also put the data in a nice plot.



- Make note of the speed up.
- Transition to  $O(3)$  model.
- I realized that vectors are continuous memory, almost no slowdown. ##  
November 11
- Updates:
  - Ran calculations again
    - \* Execution time is actually on a similar order or magnitude
    - \* MPI on 4 cores actually slows progress
    - \* A couple of outliers, checked closer, seems right
  - Redeveloped gif debugging tool for C++
    - \* Shows similar lattice for both methods.
    - \* Can be ported to  $O(3)$  model

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