# 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 algoriths. 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 dont 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 suseptibility, 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 asymtotic 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 suseptibility
  - 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:  $a \to 0$  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 regularlize: 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) opprators 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
  - nonrenormalizeable: requires infinitely many counterterms
  - super-renormalizeable: 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 transcibe 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<sup>4</sup> 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.

#### Wednesdesday, 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 attanetion
- 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]

### 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?
    - $\ast$  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
    - \* Asymtoticaly 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
- $\bullet\,$  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.

## References

- Alles, B., and A. Papa. 2007. "Numerical Study of the Mass Spectrum in the 2D O(3) Sigma Model with a Theta Term." arXiv:0711.1803 [Hep-Lat], November. http://arxiv.org/abs/0711.1803.
- Aoki, Sinya, Kengo Kikuchi, and Tetsuya Onogi. 2015. "Gradient Flow of O(N) Nonlinear Sigma Model at Large N." Journal of High Energy Physics 2015 (4): 156. https://doi.org/10.1007/JHEP04(2015)156.
- Balog, J., F. Niedermayer, M. Pepe, P. Weisz, and U.-J. Wiese. 2012. "Drastic Reduction of Cutoff Effects in 2-d Lattice O(N) Models." *Journal of High Energy Physics* 2012 (11): 140. https://doi.org/10.1007/JHEP11(2012)140.
- Horgan, R R. 2014. Statistical Field Theory.
- Hoshen, J., and R. Kopelman. 1976. "Percolation and Cluster Distribution. I. Cluster Multiple Labeling Technique and Critical Concentration Algorithm." *Physical Review B* 14 (8): 3438–45. https://doi.org/10.1103/PhysRevB.14. 3438.

Introduction to QCD and the Standard Model. n.d.

Kleinert, Hagen. 2016. Particles and Quantum Fields.

- Kleinert, Hagen, and Verena Schulte-Frohlinde. 2001. Critical Properties of  $\phi^4$ -Theories.
- Körner, Daniel. n.d. "Non-perturbative renormalization on the lattice," 124.
- Loinaz, Will, and R. S. Willey. 1998. "Monte Carlo Simulation Calculation of Critical Coupling Constant for Continuum  $\phi_2^4$ ." *Physical Review D* 58 (7): 076003. https://doi.org/10.1103/PhysRevD.58.076003.
- Makino, Hiroki, and Hiroshi Suzuki. 2015. "Renormalizability of the Gradient Flow in the 2D O(N) Non-Linear Sigma Model." Progress of Theoretical and Experimental Physics 2015 (3): 33B08–0. https://doi.org/10.1093/ptep/ptv

028.

- Makino, H., F. Sugino, and H. Suzuki. 2015. "Large-N Limit of the Gradient Flow in the 2D O(N) Nonlinear Sigma Model." *Progress of Theoretical and Experimental Physics* 2015 (4): 43B07–0. https://doi.org/10.1093/ptep/ptv 044.
- Michael, C. 1986. "Fast Heat-Bath Algorithm for the Ising Model." *Physical Review B* 33 (11): 7861–2. https://doi.org/10.1103/PhysRevB.33.7861.
- Monahan, Christopher. 2016. "The Gradient Flow in Simple Field Theories." In Proceedings of the 33rd International Symposium on Lattice Field Theory PoS(LATTICE 2015), 052. Kobe International Conference Center, Kobe, Japan: Sissa Medialab. https://doi.org/10.22323/1.251.0052.
- Monahan, Christopher, and Kostas Orginos. 2015. "Locally Smeared Operator Product Expansions in Scalar Field Theory." *Physical Review D* 91 (7): 074513. https://doi.org/10.1103/PhysRevD.91.074513.
- Morningstar, Colin. 2007. "The Monte Carlo Method in Quantum Field Theory." arXiv:Hep-Lat/0702020, February. http://arxiv.org/abs/hep-lat/0702020.
- Newman, M. E. J., and G. T. Barkema. 1999. Monte Carlo Methods in Statistical Physics. Oxford: Oxford University Press.
- Schaich, David A, and William Loinaz. 2006. "Lattice Simulations of Nonperturbative Quantum Field Theories." Amherst College.
- Tong, David. 2007. Quantum Field Theory. University of Cambridge Part III Mathematical Tripos.
- ———. 2017. Statistical Field Theory. University of Cambridge Part III Mathematical Tripos.
- Toussaint, D. 1989. "Error Analysis of Simulation Results: A Sample Problem," nos. AZPH-TH-89-72 (December): 12 p. https://cds.cern.ch/record/204810.
- Wang, Jian-Sheng. 1989. "Clusters in the Three-Dimensional Ising Model with

a Magnetic Field." *Physica A: Statistical Mechanics and Its Applications* 161 (2): 249–68. https://doi.org/10.1016/0378-4371(89)90468-8.

Wolff, Ulli. 2007. "Monte Carlo Errors with Less Errors." Computer Physics Communications 176 (5): 383. https://doi.org/10.1016/j.cpc.2006.12.001.