VIGRE REPORT PART II · SUMMER 2009

JOHN KERL

1. Sims Tucson FRG workshop · June

In June, UA's Bob Sims hosted a workshop on quantum spin systems and applications in quantum computation. I gave a talk on lattice quadrupling for percolation in quantum networks, as described in my summer/fall 2009 VIGRE proposal. In this talk, I brought my written presentation up to my current level of understanding. The remaining issues involve finite-size scaling; the only remaining obstacle to publication of this percolation work is my increasing understanding of finite-size scaling, which is hand-in-hand with FSS as applied to my dissertation research.

2. Marseille · July

I visited the Centre National pour Récherche Scientifique in Marseille during July 22-24, 2009. Daniel Ueltschi was present, having arrived a few weeks earlier; Daniel Gandolfo and Jean Ruiz were my (very gracious) hosts.

- Daniel Ueltschi presented his upcoming paper with Volker Betz, in which they obtain a cycle-weight expression for the Bose gas: namely, the α_ℓ's are chosen (using first-order approximations in scattering length a) to match the Bose-gas Hamiltonian. Daniel Gandolfo may conduct simulation efforts using these cycle weights, but not immediately: Ueltschi and Betz are still checking their work.
- Gandolfo and Ueltschi gave me valuable feedback on my slides for my upcoming Berlin talk.
- Gandolfo has a Hoshen-Koppelmann-like idea for simulating the cycle-weight model, which, if it works out, will be more efficient than my existing code. His idea would give $O(N \log N)$ complexity; mine is currently $O(N^2)$ but with a very small proportionality constant, which (I believe) suffices.
- Gandolfo's explication of the Hoshen-Koppelmann algorithm for percolation enabled me to understand what I hadn't before; I will use this for new computational work on my percolation project.
- Gandolfo gave me a better idea for computing distances on the torus.
- In spring of 2008 I found the true Bose-gas interactions to be computationally infeasible, even using lookup tables. Gandolfo points out that an angle between permutation jumps can be factored out, leading to reduced lookup-table sizes. It may be worth re-examining this.
- Gandolfo points out that the Binder fourth-order cumulant, with which I had been experimenting for finite-size scaling, is useful for first-order phase transitions whereas ours is certainly second-order.
- Ueltschi and I discussed autocorrelation. This forced me to theoretically justify my practical understand of autocorrelation; see below.
- Ueltschi points out a conjecture for the exact infinite-volume behavior of the $\mathbb{E}[f_{1,k}]$ plots. I will conduct statistical hypothesis tests against my simulation data for the Ewens model to verify this conjecture.
- Gandolfo and I will continue to stay in touch, including sharing software code; he has offered to give me feedback on the dissertation chapters I sent to him before the meeting.

Date: August 18, 2009.

3. Berlin · July

I delivered a contributed talk at the Conference on Stochastic Processes and Their Applications in July in Berlin. I had planned to present my worm algorithm for the random cycle model; on further reflection, realizing that the audience was more probabilists and fewer experimentalists, I designed a presentation which would make the random-cycle model palatable to a probabilist.

I had a productive conversation with Daniel Ueltschi's colleague Stefan Grosskinsky; with a PhD student contact of Daniel's at Potsdam I had a fruitful discussion of Ginibre's path-integral methods. Most importantly, I have an idea for a postdoc project, on minimal-distance matching of Poisson point processes. This would combine theory of Anders Holroyd (communicated to me by Tom LaGatta) with to-be-developed MCMC methods somewhat related to my current research.

4. Integration workshop · August

Friday August 7 through Tuesday August 11, I participated in the department's integration workshop for incoming graduate students. I wrote a project on the Berlekamp algorithm for factorization of polynomials over finite fields, an old area of expertise from my master's-degree days. None of the eight incoming students chose to work on that project; I assisted Angel Chavez and Kevin Davidsaver on their group-representation project, focusing in particular on presentation skills.

5. Bridge group · Early fall

Tom Kennedy's bridge group has begun meeting again for the fall as of a week ago; I have now attended two meetings. Graduate students include myself, Michael Gilbert, and Shane Passon. Four potentially interested undergraduates attended today's meeting; they will be able to participate as undergraduate research assistants for pay or for academic credit. We sketched some potential areas for involvement, and agreed to meet again next week. At this point, my hunch is that two the four undergrads will continue with the bridge group; time will tell.

My other contribution to this early point has been working with Shane on vertical integration of computational techniques, namely: makefiles, softwaare profiling (in which subroutines does one's program spend the most time?), debugging, and hands-off background execution of jobs.

6. Dissertation chapters · spring and summer

Between the submission of my VIGRE application in early April and the start of the summer, I had written the worm-algorithm and software-architecture chapters of my dissertation. This was at Daniel Ueltschi's request, to prepare for my meeting with Daniel Gandolfo as described above.

The angle-correlation question alluded to in my VIGRE proposal will not be pursued: the upper-bound and lower-bound interaction formulas of Betz and Ueltschi are far too loose to be of use.

For my Berlin presentation I began to quantify the empirical dependence of the GRU quotient $\ell_{\max}/Nf_I$ on the interaction parameter α.

7. Finite-size scaling · June

As mentioned above, finite-size scaling is needed for my disseration research as well as the percolation project. Let $t = (T - T_c)/T_c$. Given an infinite-volume quantity $S(T)$ scaling as $S(T) \sim |t|^\rho$, and a correlation length

$\xi(T)$ scaling as $\xi(T) \sim |t|^{-\nu}$, the FSS hypothesis is that the finite-volume quantity is $S_L(T) \sim L^{-\rho/\nu} Q(L^{1/\nu} t)$, where Q is a (model-dependent) universal scaling function.

For percolation, p_c (playing the role of T_c) is well-known, as is ν. Then, using an intersection method to be detailed in my dissertation, it is relatively straightforward to find ρ, which is the item of interest.

For the random-cycle model, ν and ρ must be determined experimentally, but are of only secondary interest to T_c which is the prize. After juggling half a dozen approaches over the last few months, I currently plan to find ν and ρ by extrapolation methods, then use an intersection method to find T_c.

Specifically, my next round of large-scale compute jobs, early this fall semester, will do the following:

- Make use of my recently added batched-mean code, for variance reduction.
- Use the four order parameters f_I, f_S, f_W, and $1/\xi$.
- Use a few dozen T values for $0.98 \leq T/T_c \leq 1.02$. (This is a tighter region around T_c than in previous experiments.)
- Use box size L large enough to get stable extrapolation of the critical exponents ρ and ν.
- Organize the CPU time toward getting more reliable (i.e. lower-variance) numbers over few parameter points.

8. Autocorrelations and batched means · July and August

Introductory statistics courses, at the undergraduate or graduate level, focus on the handling of IID samples. Yet, time-series data acquired in Markov chain Monte Carlo simulations tend to be highly correlated. Up until this summer, I had had a vague idea that quantification of autocorrelation was important; late last spring Tom Kennedy told me about batched means.

This summer, I have finally bitten the bullet and have gotten a handle on both these topics: I have worked out detailed calculations for (a) a particular, exactly solvable Markov chain with known autocorrelation, and (b) any Markov chain chain where $\mathrm{Corr}(X_i, X_j) = \exp(-|i-j|/\tau)$ for some scaling constant τ. The material is ready to be typed up, and will form an appendix to my dissertation. Berg's *Markov Chain Monte Carlo Simulations and Their Statistical Analysis* has proved to be a very useful reference. As well as working out the theory, I have implemented batched means in my software simulations. The theoretical understanding allows me to choose the correct batch sizes.

9. Caching of cycle lengths

A significant software optimization was a change to cache cycle lengths in a data structure separate from the lattice. The mathematical results are the same; however, the program now runs to completion in reasonable time for larger lattice sizes with Ewens interactions, which was not the case before.

10. Upcoming conferences · early 2010

The Joint Meetings of the AMS/MAA will be Jan. 13-16, 2010. I have submitted my abstract for a contributed talk on my research. I will be on the job market; AMS attendance will be key.

David Landau's Center for Simulational Physics in Athens, Georgia, will be holding a weeklong conference Mon.-Fri. Feb. 15-19 2010. Applications are not yet open; I will certainly attend. This conference looks to be the most closely aligned with my interests that I have yet attended. I hope to obtain feedback toward overcoming the stopping-time limitation of my nascent worm algorithm; I also hope to make many professional contacts.