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Critical behaviour and phase structure of 3d Scalar+Gauge Field Theories in the adjoint representation

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In a class of holographic models for cosmology, the dual theory is given by a massless super-renormalisable QFT in 3 dimensions. In order to obtain cosmological observables, correlators of this QFT may be obtained via lattice field theory. Previous work has focused on scalar ϕ^4 matrix theories in the adjoint representation of SU(N). In this work we present preliminary results in the critical behaviour and phase structure of the theory with an SU(N) scalar field coupled to gauge fields by utilising the Heatbath-Overrelaxation (HBOR) algorithm in lattice field theory.

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1. Introduction

The $3d$ SU(N) theory of adjoint scalars coupled to gauge fields is generally of interest due to being the high-temperature limit of 4d QCD [1], as well as having applications in doped cuprates [2]. This model has been extensively studied since the seminar work by Polyakov [3, 4], including [5–8]. For the purposes of the Holographic Cosmology model, however, it is conjectured that a 4d gravitational theory is dual to the massless regime (*i.e.* where it acquires a generalised conformal structure) of a superrenormalisable 3d theory of adjoint scalars and gauge fields. In this model, the two-point function of the Energy-Momentum Tensor $T_{\mu\nu}$ is related to the power spectrum of the Cosmic Microwave Background (CMB) in the gravitational theory [9, 10]. Perturbative calculations [11] show that the CMB spectrum predicted by Holographic Cosmology is competitive with ΛCDM for multipoles $l \geq 30$ [12]. However, lower multipoles reside in the nonperturbative region of the dual QFT and therefore require simulations of lattice QFT.

2. Algorithm

The theories discussed in the upcoming sections were simulated with the Grid library [13], within which a Heatbath-Overrelaxation (HBOR) algorithm was written, consisting of a HB step plus n OR steps, *i.e.* reflections. The updating of scalar fields follows the prescription in [14], with slight alterations for numerical stability. Gauge links are updated according to [15], and generalised from SU(2) to SU(N) via the subgroup method [16]. Due to the lack of fermionic degrees of freedom, the HBOR algorithm is significantly more efficient at generating decorrelated configurations than the Hybrid Monte-Carlo [17], which we used for some of our earlier simulations.

3. Adjoint Scalar SU(N) Theory

The simplest candidate dual theory for Holographic Cosmology is a ϕ^4 theory of scalars in the adjoint representation, with large-N lattice action as given below:

$$S = \frac{N}{g} a^3 \sum_{x \in \Lambda^3} \mathrm{Tr} \left\{ \sum_{\mu} [\delta_\mu \phi(x)]^2 + m^2 \phi^2(x) + \phi^4(x) \right\}, \tag{1}$$

where $\delta_\mu \phi(x) = \frac{1}{a}(\phi(x+\hat{\mu}) - \phi(x))$ and the scalar field is composed of Hermitian $N \times N$ matrices valued in the $\mathfrak{su}(N)$ algebra. A good observable with which to visualise the phase transition is the *Binder cumulant* [18]:

$$B(m^2) = 1 - \frac{1}{N} \frac{\langle \mathrm{tr}[(\sum_x \phi(x))^4] \rangle}{\langle \mathrm{tr}[(\sum_x \phi(x))^2] \rangle^2}. \tag{2}$$

The Binder cumulant is discontinuous at the continuum phase transition, and in the lattice simulation it is expected to scale next to the continuum critical point as

$$\lim_{m^2 \to m_c^2} B(m^2) \sim f\left((m^2 - m_c^2)(gL)^{1/\nu} \right), \tag{3}$$

where ν is a critical exponent of the phase transition. Apart from finding the exact position of the continuum critical point, lattice evaluations of this theory allow one to compute its critical exponents, which is important to verify in which universality class the theory lies. Massless superrenormalisable theories like the one at hand tend to be well-behaved in the UV but suffer from severe perturbative divergences in the IR. Nonetheless, it has been conjectured in [19, 20] and shown for some specific cases (for example massless scalar 3d QED) that it is possible to cure such IR divergences and prove IR-finiteness of the theory. Our collaboration has published compelling evidence [21] that indeed this is the case for the pure scalar theory. Another work investigated by our collaboration the renormalisation of the Energy-Momentum tensor ($T_{\mu\nu}$), since this is the observable whose correlator is mapped into the CMB spectrum in the dual gravitational theory of Holographic Cosmology. Because of the breakdown of translational symmetry in lattice discretisation, one cannot rely on continuum Ward Identities and the issue of renormalising $T_{\mu\nu}$ becomes nontrivial. Strides have been made by our collaboration in the pure scalar case by applying the Wilson Flow to $T_{\mu\nu}$ renormalisation [22].

4. Scalar+Gauge SU(N) Theory

If we now couple the adjoint scalars from (1) to SU(N) gauge links, we obtain the action

$$S[\phi, U] = \frac{N}{g} \sum_{x \in \Lambda^d} \mathrm{Tr} \left[a^3 \left(\sum_{\mu=1}^{d} (\Delta_\mu \phi(x))^2 + m^2 \phi^2(x) + \lambda \phi^4(x) \right) + \frac{1}{a} \sum_{\mu<\nu} \mathrm{Re} \left[\mathbb{1} - P_{\mu\nu} \right] \right], \quad (4)$$

where $P_{\mu\nu} = U_\mu(x) U_\nu(x+a\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)$ is the plaquette operator and $\Delta_\mu \phi(x) = a^{-1}(U_\mu(x)\phi(x+a\hat{\mu})U_\mu^\dagger(x) - \phi(x))$ is the gauge covariant lattice derivative in the adjoint representation. As before, $\phi(x)$ is valued in $\mathfrak{su}(N)$. The weak gauge coupling regime recovers the pure scalar case, whereas taking $\lambda \to \infty$ leads to the fixed-length scalar theory. The action given in (4) for $N = 2$ has been the subject of theoretical [7] and numerical [8] computations attempting to establish its phase diagram and the order of its transitions. It is known that, differently than in the pure scalar case, the symmetric and broken phases of the system are simply connected through a crossover region or are separated by first-order behaviour. To the authors' knowledge, so far no evidence of a second-order transition has been found, and a point (or line) between these two regimes where the continuum scalar field's mass is zero remains a conjecture. By perturbatively computing the scalar self-energy to two loops and setting the lattice spacing $a = 1$, one obtains the mass counterterm [23]

$$\begin{aligned}\delta^2_{m^2\to 0} = &-\frac{\Sigma g}{4\pi}\left[2 + \lambda\left(2 - \frac{3}{N^2}\right)\right] \\ &- \frac{1}{16\pi^2}\left[2g^2\lambda\left(2 - \frac{3}{N^2}\right)\left(-\delta + \frac{\Sigma^2}{4}\right) + g^2\left(2\kappa_1 - \kappa_4 - 4(\delta+\rho) + \pi\Sigma\left(\frac{1}{2} - \frac{4}{3N^2}\right) + \frac{5\Sigma^2}{8}\right)\right. \\ &\left.+\left(2g^2\lambda\left(2 - \frac{3}{N^2}\right) - 18 + 6N^2 - N^4\right)\left(\zeta + \log\frac{6}{\mu}\right)\right], \quad (5)\end{aligned}$$

which serves as a guide as to where, naïvely, the critical line should lie. The values of the numerical constants Σ, κ_1, κ_4, δ, ρ, and ζ in (5) are given in [23]. Investigating a region around this critical line for $\lambda = 1$, $N = 2$ and $ag < 1$, we obtain Figure 1, which shows indeed that above the perturbative critical line, especially for $ag \ll 1$, the expectation value of $\mathrm{Tr}[\phi^2]$ increases when one wades deep into the broken region, whereas below the line it remains close to zero, as would be expected of a symmetric phase. Nonetheless, this effect all but disappears when g is increased, thus suggesting the existence of crossover behaviour. The same effect is verified when analysing the scalar field's susceptibility χ across this line, as seen in Figure 2, with

$$\chi = \frac{V}{a^3}\left(\frac{\langle(\sum_x \mathrm{Tr}[\phi^2])^2\rangle}{\langle\sum_x \mathrm{Tr}[\phi^2]\rangle^2} - 1\right), \tag{6}$$

where V is the lattice volume. These figures suggest that, as expected, in the deep weak coupling regime one may recover the pure scalar behaviour. While these diagrams are preliminary, they point to strategies in finding the critical line where the scalar mass is zero, which is of relevance to our project on holographic cosmological models. It is believed that such a critical line will be located where the surface $m^2_{\mathrm{crit}}(g, \lambda)$, dividing the broken and symmetric phases through a first-order phase transition, terminates and crossover behaviour begins. Therefore, by evaluating how the susceptibility of the scalar field scales in a region of parameter space suspected of containing critical behaviour, we may distinguish these regimes by noting that, as $L \to \infty$ and $m^2 \to m^2_{\mathrm{crit}}$, we have $\chi \sim f\left(|m^2 - m^2_{\mathrm{crit}}|(gL)^{-\gamma}\right)$ along the critical line, with γ a critical exponent, whereas $\chi \sim$ const in the first-order region and $\chi \to 0$ elsewhere.

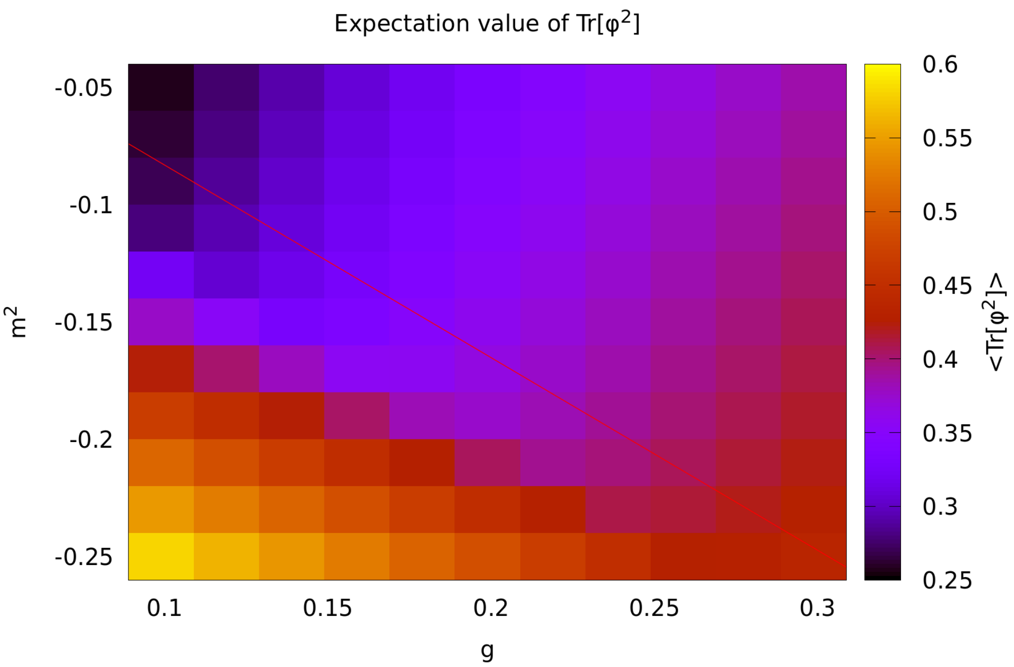

Figure 1: Expectation values of $\mathrm{Tr}[\phi^2]$ across the perturbative critical line with $N = 2$ and $\lambda = 1$ on a 64^3 lattice for various values of g and m^2. The red line indicates where critical behaviour should occur according to 1-loop lattice perturbation theory. As expected, deeper into the broken region (in this case the bottom left corner), the expectation value of $\mathrm{Tr}[\phi^2]$ increases, whereas in the symmetric region it stays close to zero.

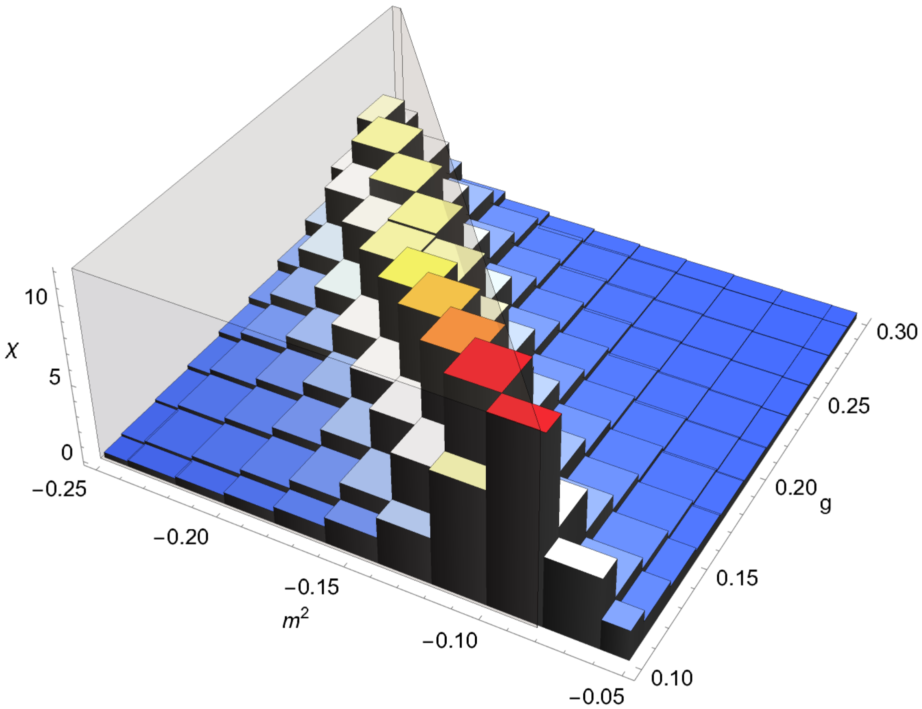

Figure 2: Expectation values of χ across the perturbative critical line with $N = 2$ and $\lambda = 1$ on a 64^3 lattice for various values of g and m^2. The grey bounding box indicates where, perturbatively to 1 loop, the broken phase lies. Across the suspected phase transition, the value of χ peaks and falls back to zero elsewhere. Scaling analysis will indicate whether this line corresponds to a first-order transition or crossover behaviour.

5. GPU Porting

Given the commissioning of the new DiRAC Tursa machine in Edinburgh, fitted with NVIDIA A100 GPUs, it became critical to port the previously CPU-based Holographic cosmology code to GPU. This was done by focusing on the main bottleneck CPU routines:

- **Lattice-wide operations**, like sum, matrix products, exponentiation, etc. Most of these operations are handled by low-level Grid routines which had already been ported to GPU, therefore optimising them amounted to porting to GPU code around them, so as to minimise memory transfer overhead.
- **Pick- and SetCheckerboard**, the former of which selects the odd or even checkerboard of the lattice and transfers that to a so-called “Red-Black" lattice with half the linear size. The latter does the inverse process. This was accelerated by creating a new Grid kernel which can translate lattice site and SIMD indices into lattice cartesian coordinates on the device. Formerly, these were methods of a host class.
- **Nearest-Neighbour interactions**, which on Grid can be performed either by Circular Shift (also known as Cshift) or stencil routines. Cshift has been recently accelerated by the Grid development team, whereas for this project stencil GPU kernels have been used and tested. The Halo Exchange part of the stencil routine is able to produce bandwidth close to 600GB/s,

which is the theoretical bandwidth of NVLink connections which are used between GPUs within the same node on Tursa.

- **RNG**, the last bottleneck routine running on host code, which is still in the process of being accelerated via device code. This requires creating an RNG class based on `curand` which can save and restore RNG states, as well as pass statistical tests of random number quality. Regarding random number quality, the `CURAND_RNG_PSEUDO_PHILOX4_32_10` RNG type on `curand` passes the BigCrush battery of statistical quality tests [24].

With the accelerated routines described above, the following improvements were verified in each of the HBOR update steps for a 256^3 lattice (Figures 3 to 6). **NB** these results do not yet include RNG acceleration, which can be seen from the fact that the RNG becomes, in some cases, the main time bottleneck.

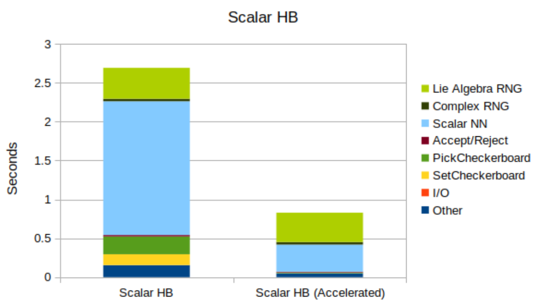

Figure 3: Scalar HB GPU acceleration

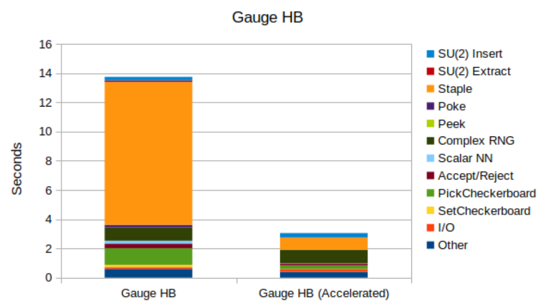

Figure 5: Gauge HB GPU acceleration

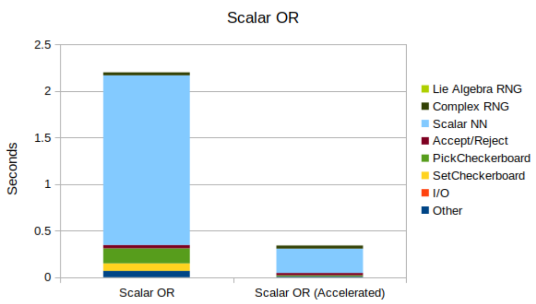

Figure 4: Scalar OR GPU acceleration

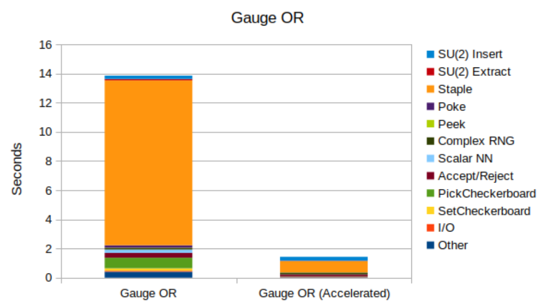

Figure 6: Gauge OR GPU acceleration

In a realistic run, however, these routines would not all hold the same weight, since the overrelaxation step needs to be performed many more times than the heatbath one. Supposing a run where we choose to have 16 OR steps for each HB, the total GPU acceleration, considering as well the time taken to save configurations and observables, is given on Figure 7. In total, for such a run, the acceleration verified is of about 87%. It must be noted that this figure is still expected to improve once the RNG acceleration has been introduced, as the GPU RNG is about one order of magnitude faster than its host counterpart.

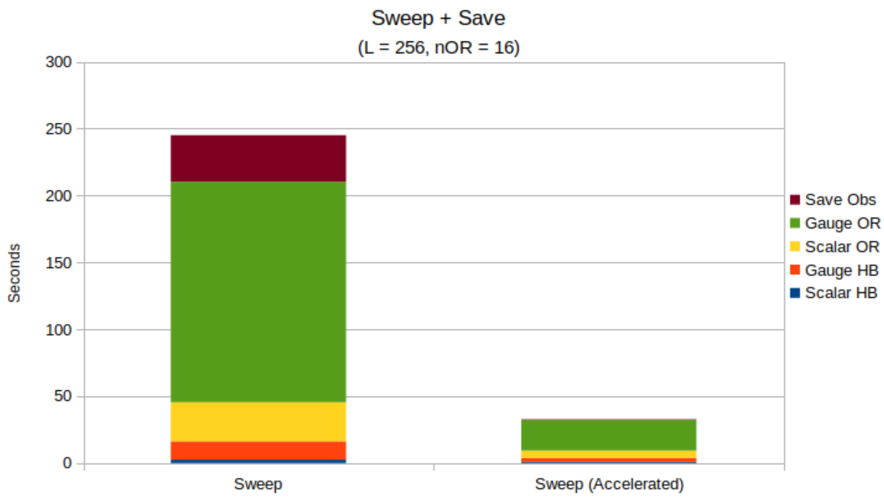

Figure 7: GPU acceleration for full HB+16OR sweep

6. Discussion

The preliminary results in this document support previous findings which demonstrate that the 3d Scalar+Gauge SU(2) theory with adjoint scalars contains regions of crossover and first-order behaviour. Furthermore, it has been established that using the Grid library, significant speedups can be achieved by using GPUs, with a realistic potential for further acceleration, once the RNG operations are also performed on the device. Future developments in this project will attempt to establish the precise line where the critical behaviour lies, and analyse the IR limit in this regime, with the aim of confirming nonperturbative IR-finiteness for the theory of interest.

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