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Katy Clough

# Scalar Fields in Numerical General Relativity

Inhomogeneous Inflation and Asymmetric  
Bubble Collapse

Doctoral Thesis accepted by  
the King's College London, UK

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# Supervisor's Foreword

The paradigmatic idea of the Big Bang for the last three decades is Inflation. In order to explain why the universe today is isotropic, homogeneous and spatially flat, the theory of Inflation posits that during the earliest moments after the birth of the Universe, there was a period of accelerated expansion, 'inflating' the Universe in size by at least 60 e-foldings (i.e.  $e^{60}$ ). Furthermore, it predicts the presence of a spectrum of nearly scale-invariant primordial perturbations—perturbations that eventually grow under gravity to form the galaxies and stars we see today. This spectrum was triumphantly discovered, imprinted as temperature anisotropies on the Cosmic Microwave Background, first by the BOOMERANG experiment in 2000 and subsequently measured in exquisite detail by many experiments thereafter. Efforts to detect the spectrum of primordial gravitational waves, also predicted by Inflation, are well underway.

Nevertheless, despite its success, Inflation faces many foundational challenges. One key challenge is whether it can actually 'begin' in the first place, in the presence of initial conditions which are not homogeneous, isotropic and spatially flat. Since its whole *raison d'être* is to explain why the current universe has these exact properties, this is a fundamentally important point for theorists to resolve.

To answer this question, one must be able to solve the non-linear Einstein equations, with initial conditions that exhibit very little symmetry. This is an extremely difficult task that is not tractable analytically, and until recently, not tractable even numerically. Indeed, for most of Inflation's existence as a theory, almost all models have assumed that this issue is 'magically solved', or at least, unsolvable until such time as we have developed both sufficient theoretical know-how and computational technology. That time is now. Recent advances in numerical relativity—the computational solution of the Einstein equations of gravitation—driven largely by efforts to detect gravitational waves, have now reached sufficient sophistication and maturity to allow these fundamental questions to be attacked.

Dr. Clough's thesis represents the vanguard of these attempts at understanding the beginnings of Inflation, and hence of the modern Big Bang theory. In her groundbreaking thesis, she demonstrated, for the first time, that Inflation can fail to

begin, particularly in the so-called ‘small field’ case preferred by string theory models. On the flipside, she also demonstrated, again for the first time, that inflation can begin even if some part of the universe is initially collapsing. In order to do this, she developed the necessary code, and theoretical intuition, which forms the basis of her current post-doctoral research. While working on the science, Dr. Clough also played a key role in the development of the numerical relativity code, GRChombo, which is used extensively in her thesis work.

Theoretical physics in recent decades have become highly competitive and specialised, and the increasingly long journey to reach the frontier of physics research often limits the ambition of many Ph.D. theses. Dr. Clough’s thesis is a brilliant exception to this rule—it is trailblazing in its potential to open up a new field of study in cosmology. I am, hence, incredibly pleased, and proud that this brilliance is recognised by a Springer Theses award.

London, UK  
March 2018

Dr. Eugene Lim

# Abstract

Einstein’s field equation of General Relativity (GR) has been known for over 100 years, yet it remains challenging to solve analytically in strongly relativistic regimes, particularly where there is a lack of a priori symmetry. Numerical Relativity (NR)—the evolution of the Einstein Equations using a computer—is now a relatively mature tool which enables such cases to be explored. In this thesis, a description is given of the development and application of a new NR code, GRChombo.

GRChombo uses the standard BSSN formalism, incorporating full Adaptive Mesh Refinement (AMR) and massive parallelism via the Message Passing Interface (MPI). The AMR capability permits the study of physics which has previously been computationally infeasible in a full  $3 + 1$  setting. The functionality of the code is described, its performance characteristics are demonstrated, and it is shown that it can stably and accurately evolve standard spacetimes such as black hole mergers.

We use GRChombo to study the effects of inhomogeneous initial conditions on the robustness of small and large field inflationary models. We find that small field inflation can fail in the presence of subdominant scalar gradient energies, suggesting that it is much less robust than large field inflation. We show that increasing initial gradients will not form sufficiently massive inflation-ending black holes if the initial hypersurface is approximately flat. Finally, we consider the large field case with a varying extrinsic curvature  $K$ , and find that part of the spacetime remains inflationary if the spacetime is open, which confirms previous theoretical studies.

We investigate the critical behaviour which occurs in the collapse of both spherically symmetric and asymmetric scalar field bubbles. We use a minimally coupled scalar field subject to a ‘double well’ interaction potential, with the bubble wall spanning the barrier between two degenerate minima. We find that the symmetric and asymmetric cases exhibit Type 2 critical behaviour with the critical

index consistent with a value of  $\gamma = 0.37$  for the dominant unstable mode. We do not see strong evidence of echoing in the solutions, which is probably due to being too far from the critical point to properly observe the critical solution.

We suggest areas for improvement and further study, and other applications.



# Acknowledgements

I would like to sincerely thank my supervisor, Eugene Lim, for giving me the opportunity to pursue a career in research. I am grateful in particular for his support, encouragement and invaluable advice during the Ph.D. His contributions run throughout the work presented in this thesis, over and above his significant role as co-author on the papers presented in Chaps. 3–6.

I am also grateful for the contributions of my GRChombo collaborators, Hal Finkel, Pau Figueras, Markus Kunesch and Saran Tunyasuvunakool, for their work on the code development and testing, in particular in relation to the scaling and convergence tests presented in Chap. 3. Moreover, I would like to thank them for their various useful insights and discussions, and for being a great team to work with—always willing to share ideas and knowledge. I look forward to continuing our collaboration in future, particularly on the new version of the code, for which Saran and Markus in particular deserve credit for their work alongside Intel.

Also in relation to the work presented in Chap. 3, I would like to thank the Lean collaboration for allowing us to use their code as a basis for comparison, and especially Helvi Witek for helping with the setting up and running of the Lean simulation. I would like to thank Juha Jaykka, James Briggs and Kacper Kornet at DAMTP for their amazing technical support. The majority of the work in this thesis was undertaken on the COSMOS Shared Memory system at DAMTP, University of Cambridge operated on behalf of the STFC DiRAC HPC Facility. This equipment is funded by BIS National E-infrastructure capital grant ST/J005673/1 and STFC grants ST/H008586/1, ST/K00333X/1. The research also used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility, supported under Contract DE-AC02-06CH11357, and I benefitted greatly from attending their ATPESC 2015 course on supercomputing. I also used the ARCHER UK National Supercomputing Service (<http://www.archer.ac.uk>) for some simulations, and again, attended a number of their courses on High Performance Computing which I found invaluable. Part of the performance testing was performed on Louisiana State University’s High Performance Computing facility.

I would like to acknowledge my co-authors on the paper ‘Robustness of Inflation to Inhomogeneous Initial Conditions’, presented in Chap. 4, in particular Raphael Flauger, for his deep knowledge of the topic of inflation, but also Brandon S. DiNunno, Willy Fischler and Sonia Paban. I am grateful to William East for sharing with us details of his simulations, and to Jonathan Braden, Hiranya Peiris, Matt Johnson, Robert Brandenberger, Adam Brown and Tom Giblin for useful conversations on this and related projects.

In Chap. 6, I briefly present work I was involved in for the paper ‘Black Hole Formation from Axion Stars’, carried out with Thomas Helfer, David J. E. (Doddy) Marsh, Malcolm Fairbairn and Ricardo Becerril. I acknowledge their contributions but in particular Thomas for doing most of the hard work on the simulations and Doddy for his encyclopaedic knowledge of axions.

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# Nomenclature

## Roman Symbols

$\mathbf{u}$	The state vector (an ordered list of the evolution variables, rather than a geometric vector)
$\mathbf{w}$	The vector of eigenfunctions $w$ (an ordered list, rather than a geometric vector)
$\hbar$	Reduced Planck's constant
$\mathcal{H}$	The Hamiltonian constraint
$\mathcal{L}$	Langrangian density
$\mathcal{L}_{\mathcal{G}}$	Langrangian density for the Einstein–Hilbert action
$\mathcal{L}_{\mathcal{M}}$	Langrangian density for a matter field
$\mathcal{L}_{\mathcal{SF}}$	Langrangian density for a scalar field
$\mathcal{M}$	A manifold
$\mathcal{M}^i$	The momentum constraints
$\mathcal{N}$	In cosmology, the number of e-folds
$\tilde{D}_i$	The metric compatible covariant derivative with respect to the conformal metric $\tilde{\gamma}_{ij}$
$\tilde{A}_{ij}$	The traceless part of the extrinsic curvature in the BSSN decomposition
$\tilde{R}_{ij}$	The part of the Ricci tensor related to the conformal metric
$\vec{a}$	The acceleration of the normal observers
$\vec{V}, V^a$	An arbitrary vector
$a$	In cosmology, the scale factor
$a, b, \dots$	Low counting Latin indices denote abstract tensor indices which run through 0, 1, 2, 3
$a_*$	In inflation, the scale factor when the gradient energy becomes subdominant
$A_i$	Spatial derivative of the lapse, used in stability analysis of Sect. <a href="#">2.2.2</a>
$a_{tt}$	In inflation, the scale factor at the free fall timescale
$B^i$	An auxiliary vector field used in the gamma-driver shift condition, related to the time derivative of the shift

$B_{ij}$	The magnetic part of the Weyl tensor
$c$	Speed of light in a vacuum
$C_{abcd}$	The Weyl tensor
$D_a$	The covariant derivative defined with respect to the spatial metric $\gamma_{ab}$
$d_{ijk}$	Spatial derivative of $\gamma_{ij}$ , used in stability analysis of Sect. 2.2.2
$dl$	The distance within the spatial hypersurface
$ds$	The spacetime distance
$E_{ij}$	The electric part of the Weyl tensor
$f_a$	The symmetry breaking scale for the PQ-field (for axions)
$G$	Newton's gravitational constant
$g$	Determinant of the four-dimensional spacetime metric
$G_{ab}$	The Einstein curvature tensor
$g_{ab}$	The four-dimensional spacetime metric
$H$	In cosmology, the Hubble parameter
$h_+$	In gravitational waves, the strain for the + polarisation
$h_\times$	In gravitational waves, the strain for the $\times$ polarisation
$H_s$	The symmetrising matrix of $P_s$
$i, j, \dots$	High counting Latin indices denote spatial component indices which run through 1, 2, 3
$J_{ADM}^i$	The ADM angular momentum of a spacetime
$K$	The trace of $K_{ab}$ , i.e. $g^{ab}K_{ab}$ , also $\gamma_{ij}K_{ij}$ in the adapted basis
$k$	In inflation, the wave number of the fluctuations $2\pi/L$
$k_c$	In cosmology, the curvature parameter for space
$K_{ab}$	The extrinsic curvature tensor
$K_{ij}$	The extrinsic curvature (in the adapted basis)
$k_{wall}$	In bubble collapse, the parameter defining the steepness of the bubble wall
$L$	Length of the numerical grid, in cosmology equal to $1/H$
$l$	In GRChombo, the refinement level
$M$	The mass of a black hole or compact object
$m$	The field mass, in an $m^2\phi^2$ potential
$M^i$	The characteristic matrix for the $i$ th spatial direction
$m_a$	The axion mass defined from the potential as $\Lambda_a^2/f_a$
$M_N$	In inflation, the Nariai mass of a black hole
$M_{ADM}$	The ADM mass of a spacetime
$N$	In inflation, the total number of modes of spatial fluctuations in the scalar field
$n^a$	The unit normal vector to the spatial slice, also the 4-velocity of the normal observers
$P$	Pressure (of a fluid, say)
$p$	The critical collapse parameter, with critical value $p^*$
$p^a$	4-momentum (of a fluid, say)
$P_b^a$	The projection operator for the spatial hyperslice
$P_{ADM}^i$	The ADM linear momentum of a spacetime

$P_s$	The principle symbol matrix
$R$	The Ricci scalar
$r$	Radial coordinate distance from the centre of the computational grid
$R_{bcd}^a$	Riemann curvature tensor
$R_{ij}^\chi$	The part of the Ricci tensor related to the conformal factor
$R_0$	In bubble collapse, the initial radius of the bubble wall
$R_s$	The matrix of eigenvectors of $P_s$
$R_S$	The Schwarzschild radius
$R_{ab}$	The Ricci tensor
$R_{ij}$	The three-dimensional Ricci tensor (in the adapted basis)
$S$	The trace of $S_{ij}$ , i.e. $\gamma_{ij}S_{ij}$
$s(\mathbf{u})$	Source terms in the evolution system for $\mathbf{u}$
$S^i$	The momentum density as measured by normal observers
$s^i$	Outward pointing normal vector to a 2D surface within the spatial hypersurface
$S_G$	The Einstein–Hilbert action
$S_{ij}$	The spatial part of the energy momentum tensor in the adapted basis
$T$	In critical collapse, proper time of a central observer, measured backwards from the critical time
$t$	Coordinate time, conformal time in cosmology
$T_{ab}$	The Energy Momentum (EM) tensor or stress energy tensor
$U^a$	4-velocity (of a fluid, say)
$V(\phi)$	Scalar field potential
$V^\mu$	The components of an arbitrary vector $\bar{V}$
$w_i$	In cosmology, the state parameter for a component $i$ defined by $w_i = P/\rho$
$x^i$	Coordinates of a point on the computational grid
$X_{ij}^k$	Combination of evolution variables, used in stability analysis of Sect. 2.2.2
$X_{ph}$	In cosmology, the particle horizon
$Y_{l:m}(\theta, \phi)$	The $(l, m)$ spherical harmonic
$Z$	In critical collapse, a scale-invariant variable
$z$	In cosmology, redshift

## Greek Symbols

$\alpha$	The lapse
$\beta^a$	The shift vector (in a general basis)
$\beta^i$	The (spatial components of the) shift vector
$X$	The conformal factor of the spatial metric in BSSN, defined as $x = (\det \gamma_{ij})^{-1/6}$
$\Delta\phi$	In inflation, the amplitude of the spatial fluctuations in the scalar field
$\delta\phi$	In cosmology, the distance the inflaton rolls during inflation
$\delta_j^i$	The Kronecker delta



$\Delta_R$	In inflation, the scalar power spectrum
$\Delta_S$	In critical collapse, the scale-echoing constant
$\epsilon$	In cosmology, the first Hubble slow roll parameter
$\epsilon_v$	In cosmology, the first potential slow roll parameter
$\epsilon_{ff}$	In regriding, the fill factor threshold
$\epsilon_{ijk}$	The three-dimensional Levi–Civita symbol
$\eta$	In cosmology, the second Hubble slow roll parameter
$\eta_V$	In cosmology, the second potential slow roll parameter
$\eta_{\beta i}$	Parameters in the gamma-driver shift condition, $i = 1, 2$
$\eta_{ab}$	The Minkowski metric
$\gamma$	The determinant of the three-dimensional spatial metric
$\Gamma_{\mu\nu}^\rho$	Four-dimensional Christoffel symbols
$\Gamma_{jk}^i$	The three-dimensional Christoffel symbols associated with the metric
	$\gamma_{ij}$
$\gamma_S$	In critical collapse, the scaling exponent
$\gamma_{ab}$	The spatial metric (in a general basis)
$\gamma_{ij}$	The three-dimensional spatial metric (in the adapted basis)
$\Lambda$	In cosmology, the cosmological constant
$\lambda$	The affine parameter of a curve
$\lambda_0$	In critical collapse, the eigenvalue of the growing mode
$\Lambda_a$	Parameter used in defining the shape of the axion potential
$\Lambda_s$	The matrix of eigenvalues of $P_s$
$\mu, \nu, \dots$	Greek indices denote spacetime component indices which run through 0, 1, 2, 3
$\mu_{xi}$	Parameters in the alpha-driver lapse condition, $i = 1, 2, 3$
$\mu_{\beta i}$	Parameters in the gamma-driver shift condition, $i = 1, 2$
$\nabla_a$	Four-dimensional covariant derivative
$\Omega_i$	In cosmology, the dimensionless density parameter for a component
$\phi$	Scalar field
$\phi^*$	In inflation, the minimum of the potential, corresponding to the end of inflation, and start of reheating
$\phi_0$	In inflation, the average initial position of the scalar field in field space
$\phi_m$	In bubble collapse, the location of the minima in field space
$\pi^{ij}$	The conjugate momenta of the spatial metric fields
$\Pi_M$	(minus) the conjugate momentum of the scalar field $\phi$
$\Psi$	The Newtonian gravitational potential
$\Psi_4$	The Newman Penrose scalar
$\psi_{l,m}$	The multipole components of the Weyl scalar
$\rho$	Energy density
$\rho_{crit}$	In cosmology, the critical density of the universe for $k_c = 0$
$\sigma$	The Kreiss–Oliger dissipation parameter
$\sigma_S$	In critical collapse, the logarithm of the spacetime scale
$\sigma_{tt}$	In regriding, the tagging threshold
$\sigma_{wall}$	In bubble collapse, the tension in the bubble wall

$\tau$	Proper time (in cosmology, as measured by a comoving observer)
$\Theta$	In the apparent horizon finder, expansion of the outgoing null geodesics
$\tilde{\Gamma}^i$	The conformal connection coefficients in the BSSN decomposition
$\tilde{\Gamma}^i_{jk}$	The three-dimensional Christoffel symbols associated with the conformal metric $\tilde{\gamma}_{ij}$
$\tilde{\gamma}_{ij}$	The conformal metric in the BSSN decomposition
$\tilde{d}\phi$	An arbitrary one-form
$\varphi$	The complex PQ-field (for axions)
$\xi$	In inflation, the kinetic part of the energy density for the field
$\zeta$	In bubble collapse, parameter defining the shape of the potential $V(\phi)$
$n_s$	In inflation, the spectral index
$s$	In bubble collapse, parameter defining the shape of the potential $V(\phi)$

## Other Symbols

$\mathbb{R}^n$	The real numbers
$\mathfrak{L}_{\vec{v}}$	The Lie derivative along the vector field $\vec{V}$

## Acronyms/Abbreviations

ADM	Arnowitt, Deser, Misner
AMR	Adaptive Mesh Refinement
BH	Black Hole
BSSN	Baumgarte, Shapiro, Shibata, Nakamura
CMB	Cosmic Microwave Background
CP	Critical Point
CS	Critical Surface
CSS	Continuous Self Symmetry
CTS	Conformal Thin Sandwich
CTT	Conformal Transverse Traceless
DE	Dark Energy
DM	Dark Matter
DSS	Discrete Self Symmetry
EEP	Einstein Equivalence Principle
EM	Energy Momentum (tensor)
EOM	Equation of Motion
ESA	European Space Agency
FRW	Friedmann–Robertson–Walker(–Lemaitre)
GHC	Generalised Harmonic Coordinates
GR	General Relativity
KE	Kinetic Energy
MHD	Magnetohydrodynamics
MPI	Message Passing Interface—parallel programming method

NR	Numerical Relativity
PDE	Partial Differential Equation
QCD	Quantum Chromo Dynamics
QFT	Quantum field theory
RK4	Runge–Kutta 4th order
SEC	Strong Energy Condition
SEP	Strong Equivalence Principle
SF	Scalar Field
SR	Special Relativity
VEV	Vacuum Expectation Value