

# Historical Reflections on the Role of Numerical Modeling in Astrophysics

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## 1 Introduction

It is a great pleasure to be asked to address this group at this particular university and a very special honor for me to accept here the Karl Schwarzschild Award for 1999. The specific scientific tradition embodied by Goettingen has always been the one that I was most attracted to, not just in some vague symbolic fashion but in its most personal expression. First, and most obviously, I am honored to be in the company of prior awardees, several of whom have been my colleagues at Princeton. In fact, most of my closest mentors, from my thesis advisor at Chicago, Subramanian Chandrasekhar, to my post doctoral advisor at Cambridge, Donald Lynden-Bell, and, of course, including an important mentor at Princeton, Martin Schwarzschild, are on the short list of Karl Schwarzschild Lecturers.

On my recent journey to Goettingen, I took a geographically circuitous, but historically direct, trip to this university, stopping first for two days in Potsdam, where I was able to visit the house where Martin Schwarzschild was born and from which Karl Schwarzschild was Director of the Observatory. As I noted earlier, Martin, a man for whom my personal admiration was unbounded, was the principal reason that I went to Princeton in 1965 and have stayed ever since. He, with Lyman Spitzer, created an extraordinary atmosphere of collegiality and intense scientific inquiry, an atmosphere that I have never seen matched elsewhere.

Martin, of course, received his Ph.D., from Goettingen (in 1935) where the tradition of numerical astrophysics was born. When I first met him, I did not know that his uncle (on his mother's side) was Robert Emden whose book *Gaskugeln* was the first scientific book I read in astronomy, and one I greatly admired. In fact, an early paper that I wrote in graduate school was entitled "Cylindrical Emden and Associated Functions", and I was very proud

to have found an analytic solution to the isothermal cylinder. (As an aside, I note that Spitzer found the analytic solution to the isothermal slab, but no one has yet ever found the solution, in closed form, for an isothermal sphere.)

Astronomy was perhaps the first quantitative intellectual discipline (aside from mathematics itself). Perhaps the first quantitative prediction based on natural laws was that of the return of Halley's Comet in 1759. This event firmly established in the popular mind the validity of Newton's laws. To this date, the benchmark of scientific discourse is, paradoxically, the ability to be wrong. It might have eventuated that Halley's Comet did not return to its scheduled place in the heavens at the scheduled time, thus falsifying Newton. Many scientific predictions have been false (I am the author of more than one), thus invalidating the theory which generated the prediction. But, what theologian or philosopher or historian or literary critic has been proved wrong? Falsifiability is simply not possible, not conceivable, without quantitative prediction.

The German school has exemplified the quantitative, testable, predictive power of theoretical astrophysics. From Karl Friedrich Gauss through Albrecht Unsöld, Rudolph Kippenhahn and others too numerous to mention, this tradition has been maintained as a bulwark of our profession. As but one example, the cover of the latest annual report of the Max Planck Institute for Astronomy displays a picture of a numerical simulation (not a photograph taken from observations), and perhaps one-half of the papers contained therein are in a similar spirit. This field of work is booming – it undergirds all of astrophysics – and it has become almost too successful, with the rapid development of computers. Let me now turn to a personal, and no doubt partisan, account of the character, the strengths and weaknesses of this field.

## 2 Numerical Astrophysics: Uses and Abuses

I will take examples from fields within which I have worked or I have followed closely: stellar and interstellar astronomy, stellar dynamics and cosmology.

**A) PHYSICAL MODELLING: Numerical studies serve the prosaic but extremely important role of allowing us to link observations through well-established theories, to factual information that we seek.** Examples follow:

1) Our estimates for the relative abundances of the chemical elements in astronomical objects arise from modelling either stellar absorption spectra or emission spectra from gaseous nebulae.

2) We model stellar evolution, comparing with observations to obtain estimates of the mass, age and internal composition of the observed stars.

This is the bread and butter of astronomy, without which observational results are useless. When the theories are old and very well established and the mathematical methods are well tested and customary, we even forget that we are performing an exercise of physical and mathematical modelling. We

say that we “observe” the temperature of a star or its mass when really we are doing no such thing: we are observing a spectral distribution or a light curve and inferring a temperature or a mass.

**B) NUMERICAL MODELLING: There are many problems for which we believe that we know the equations governing the phenomenon but cannot guess the solutions, and, as the equations are nonlinear and time-dependent, our analytical methods fail. Then the computed numerical solutions tell us something new – and can enlarge our understanding.**

1) Martin Schwarzschild was surprised in the late 1950s to learn that chemical discontinuities in evolved stars produced the red giant phenomena.

2) The numerical evolution of N-body systems showed the phenomena of core collapse, gravo-thermal oscillations and other phenomena which were ultimately understood by more analytical modelling.

3) Current numerical work on the dynamical formation of dark matter halos, being done by many groups around the world, is leading us – by halting steps – to an understanding of how an initial spectrum of cosmic perturbations is transformed into the large (and small) scale structures observed in the universe.

**C) SIMULATION: Here we know much but not all of the physics involved and wish to determine which elements of our understanding are important, which are not, and what are the missing ingredients in our recipe for the phenomenon.**

1) In trying (so far without perfect success) to understand Type II Supernovae, we include or exclude neutrinos, rotation or magnetic fields in various combinations to determine what is needed.

2) In trying to understand the persistence of cold molecular clouds over timescales long compared to the cooling and free fall times of these objects, we include or exclude UV and wind feedback from stars, cosmic rays and magnetic fields.

3) In cosmology, to understand where and when galaxies form, we may employ only gravitational forces (associating galaxies with halos) or attempt to model gas dynamics, cooling, feedback from star formation, etc.

In this area of simulation, there will inevitably be many free parameters and one must distinguish as carefully as possible between the precision of the results (how closely the conclusions follow from the assumptions) and accuracy (the validity with which nature has been modelled).

A word now on the overall utility of numerical treatments of the three schematic types described above. If – as is usual – one is concerned about too little accuracy, the tests which we must make in categories (A) and (B) are for convergence (as numerical modelling is refined) and for agreement among the modellers. For simulations of type (C), it is robustness that is our guide to how the results depend on uncertainty of the physical processes treated,

the parameters adopted or the numerical methods utilized. However, there is the opposite and paradoxical problem (luckily encountered very rarely) of too much accuracy. If we had essentially perfect information about the earth's atmosphere at some time and perfect knowledge of all geophysical and astronomical inputs, we could presumably model the weather to any desired degree of accuracy. But it would tell us nothing that we would not learn by waiting to see what weather actually ensued. Our understanding of nature is not increased by the perfect simulation. On the contrary, our analytical understanding of Rossby waves, convective instabilities, and Kolmogorov turbulence comes from simpler problems where we model a few characteristics of fluid flow and ignore others. Paradoxically, only approximate treatments convey information!

A word now on technical progress may be in order. In approximately 1850, hand calculations allowed C. F. Gauss to integrate one particle orbit as a function of time. One century later, around 1950, Martin Schwarzschild was able to integrate – using the first electronic computers – the evolution of a spherical star, a function of one variable and time. By the time of my Ph.D. thesis in 1965, I was able to very roughly estimate the evolution of a contracting, rotating star, involving two spatial dimensions and time. By one decade later, around 1975, Simon White, Mark Davis and others were able to perform cosmological computations involving three spatial dimensions and time – but very simple physics. Now, at the turn of the century, 2000, 3-D, time dependent calculations are beginning to be made which include gravity, full hydrodynamics, atomic physics and simplified radiative transfer.

This progress has been partly algorithmic but partly due to the justly famous “Moore’s Law”, the seemingly unstoppable ability of technological progress to effectively double the capacity of computers every eighteen months. But now, at the present era, starting from the current base of fully 3-D calculations with good physical modelling and fairly good spatial resolution, it is difficult to predict where Moore’s Law will take us. The prospects are truly awesome.

### 3 Galaxy Formation and Numerical Cosmology<sup>1</sup>

#### A) Introduction

There exists a well-defined theoretical paradigm for the development of structure in the universe. I will focus here on the “Cold Dark Matter” family of models, which have been extraordinarily successful in the last decade in helping us to comprehend a vast range of cosmological data. After an early inflationary period, the details of which remain obscure [Ref. #1], during which quantum fluctuations in a flat universe were stretched out to the point where wavelengths at the horizon scale always had the same finite but low amplitude (now known empirically to correspond to  $(\delta\rho/\rho)_{ct} \approx 10^{-5}$ ), all am-

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<sup>1</sup>Based on Ostriker, J. P. 2000, *Physica Scripta*, T85, 164–167

plitudes grew due to gravitational instability in a predictable fashion. With three components of matter – radiation (including neutrinos), baryons, and some collisionless dark matter – the method for determining the growth of structure through the phase of decoupling involves straightforward integration of a coupled set of linear differential equations for the amplitudes of the (noninteracting) Fourier modes [Ref. #2], using standard physics. In principle, integration of these equations forwards to the present time is merely an engineering problem, so that any hypothesized initial state can be evolved to the present and then compared to abundant current observations to test if the proposed model is acceptable.

Is this a well defined exercise? One might imagine the question to be well posed, if the number of “free” – adjustable – parameters were less than the number of independent observational constraints. But, in fact, it is not so simple to do this objectively, as there is a slipperiness in the definitions, and one is forced to distinguish between “parameters” and “free parameters”. An example is perhaps helpful. The Hubble constant (conventionally written as  $h \equiv H_0/100 \text{ km/s/Mpc}$ ) is so well determined by a variety of independent methods that most observers would be surprised if it were not within the range  $h = 0.65 \pm 0.10$  [Ref. #3, #4]. Similarly, the value of the baryon density in units of the critical density is usually quoted now with the very low uncertainty of  $\Omega_b h^2 = 0.019 \pm 0.01$  [Ref. #5] (primarily) from measurements of deuterium in QSO absorption spectra and standard big bang nucleosynthesis. Accepting these values, the perturbation spectrum shape can be computed at, say, decoupling with input of spectral index  $n$  (expected, from fundamental theory, to be close to unity) and the value of  $\Omega_{matter}$  (and the assumption of flatness  $\Omega_{matter} + \Omega_{rad} + \Omega_{\Lambda} = 0$ , where allowance has been made for a possible cosmological constant). Thus, given our assumptions concerning the model and the present good experimental determinations of certain quantities, the “free” parameters are reduced, for variants of the cold dark matter paradigm, to three:  $\Omega_{matter}$ , spectrum amplitude, spectral index.

Then, if two points in the power spectrum are determined observationally, we are reduced to a one parameter family of CDM-like models, dependent only on  $\Omega_m$ . The two tie-down points are provided at extrema – the longest observable spatial wavelength, where the COBE satellite fixes the quadrupole amplitude of the CBR field, and the comoving wavelength about 300 times smaller, which determines the properties of the largest observed highly nonlinear structures, the clusters of galaxies. Both amplitudes are known to about 8% (1 Sigma) comparable to the other “determined” parameters. By this chain of logic, we are reduced to a one parameter sequence of models, dependent only on  $\Omega_{matter}$  – *within a given scenario* – in this case the assumption of a flat CDM model with a (possible) cosmological constant. Then, within this framework, one can (adopting all the stated constraints) vary the input value of  $\Omega_{matter}$ , compute in as much nonlinear detail as present numerical techniques permit all the consequences of the model, compare with observations and thus “determine” the best fit value of  $\Omega_{matter}$ .

This was essentially the procedure adopted by Ostriker and Steinhardt 1995 [Ref. #6], which led to the best fit “concordance” model which proposed the parameters  $\Omega_m = 0.35$ ,  $\Omega_\Lambda = 0.65$ ,  $h = 0.70$ ,  $\Omega_b = 0.040$ ,  $\sigma_8 = 0.85$ ,  $n = 1.00$  a result updated in Wang *et al.* [Ref. #7] to  $\Omega_m = 0.33$ ,  $\Omega_\Lambda = 0.67$ ,  $h = 0.65$ ,  $\Omega_b = 0.041$ ,  $\sigma_8 = 0.90$ ,  $n = 1.00$ . At the time of the 1995 paper, the reported, preliminary Supernova I results disagreed at the two sigma level with this model. These results appeared to indicate  $\Omega_\Lambda < 0.3$ . At the present time, the supernova results appear to agree well [Ref. #7] with this LCDM model.

Before one jumps to the conclusion that cosmology is a solved problem, one must return to the italicized phrase, that one has only one truly free parameter, which can be determined by matching computation and observation *within a given scenario*. Outside of this scenario, other models may also be possible. Thus, isocurvature models may still be viable [Ref. #8], possibly hot dark matter scenarios [Ref. #9] (although I, personally, find this improbable), or, quite plausibly, other paradigms not yet conceived of. While the LCDM model (and quintessence variants) at present seem most consistent with the full panoply of observational constraints, as we all know, consistency is not proof!

Let me turn now to areas where I think the rapidly developing numerical simulations have the most to offer in sharpening the questions, in providing understanding, and, potentially, in discriminating among models.

## B) Numerical Cosmology

A first question we must ask is which one of the issues noted above do we wish to address. If our interest is in what I shall caricature as the “astronomical” side of the coin and we wish to “explain” the observed properties of the universe, the regularities observed in the characteristics of galaxies, clusters and the intergalactic absorption systems, then we seek the most robust predictions of the models, those which depend *least* on the specific scenarios. If, on the other hand, we are interested in the “cosmological” side of the issue and we wish to discriminate best amongst scenarios, then we will try to compute the *most* sensitive features, those which depend most on the specific model.

As noted earlier, models for the growth of structure are mathematically precise. The initial conditions are unknown to us and are dependent on poorly understood fundamental physics. However, the subsequent developments (given the initial conditions) can be calculated, in principle, to arbitrary accuracy using well verified physical laws and numerical techniques. In fact (as contrasted to “in principle”), a lack of sufficient computing power and of codes which incorporate a sufficiently broad suite of standard physics has, until recently, restricted work to those aspects of the problem which are dominated by a collisionless, hypothetical “dark matter”, acting only through Newton’s laws of motion and gravity. Recent technical developments allow one to make more realistic models. The problems amenable to treatment with currently available techniques include a) prediction of gravitational lensing,

b) the properties and evolution of the Lyman-alpha clouds, and c) the properties and evolution of clusters of galaxies (especially X-ray properties). These model-dependent predictions can be compared with a rapidly growing base of observations, in order to discriminate amongst proposed models. Even in these limited areas, the uncertainties in the current generation of simulations are considerably larger than the observational uncertainties. But, numerical accuracy is improving rapidly: the standard resolution ( $N \equiv$  number of resolution elements per simulation) in published work having gone from  $30^3 = 10^{4.4}$  to over  $300^3 = 10^{7.4}$  volume elements over the last five years. The present state-of-the-art for hydrodynamical simulations is  $768^3 = 10^{8.6}$  volume elements, with  $1024^3 = 10^{9.0}$  reachable within one year. Galaxy formation itself, perhaps the most important and challenging problem, appears to be beyond the capabilities of present techniques, in part because it reduces to the currently unsolved problem of star formation. We can estimate when and where galaxies will form but can only guess about their detailed properties. However, for the other areas mentioned above, we are at or near the level of resolution required to address interesting problems.

The objects most amenable to reliable computation are picked because their formation and structure can be understood via straightforward physics that does not involve the unknown physics of star formation. Understanding the formation and evolution of these entities has progressed rapidly in the last few years, so that comparison between observations and model computations is beginning to effectively weed out the less successful models. Let us now summarize the situations when model calculations can be effectively used to confront observations.

1) Dark-matter-only simulations:

a) The computed quantity must be *directly* derivable from the potential fluctuations, as these are determined largely by the dark-matter component. Thus, one might examine:

i) Gravitational lensing which measures potential fluctuations (integrated along the line-of-sight) directly.

ii) The velocity field, ranging from moments of the galaxy pairwise velocities to numbers of clusters having differing velocity dispersions, to large-scale velocity fields.

b) The computed quantity must be dominated by mass clumping on scales larger than 10 kpc, since, on small scales, the condensed (stellar) baryonic component is gravitationally significant. This eliminates, for instance, small-scale (less than 2 arcsec) gravitational lens splittings or galactic rotation curves as candidates for accurate computation.

2) Cosmological hydro simulations:

a) Most of the baryonic component should be in the gaseous, not condensed (*e.g.*, stellar) state, so that uncertainties in the conversion of gas to stars or galaxies are not important.

b) The principal processes for heating and cooling the gas are either computable, in a self-consistent fashion (*e.g.*, shock heating), or constrained by observations (*e.g.*, the UV and soft X-ray backgrounds), so that the physical state of the gas can be determined with confidence.

c) The dynamical range for the computations must be sufficient to more than bridge the gap from a resolution scale of  $\Delta L$ , less than the Jeans' length, to a box size  $L$ , large enough to provide a fair sample for the structures being studied.

At the present time, with present hardware and software, the X-ray clusters and the Lyman-alpha clouds both (marginally) satisfy these requirements for phenomena that can be investigated.

Recent work [*e.g.*, Ref. #10] has shown that modeling the Lyman-alpha clouds is pretty clearly an "astronomical success" in that the computations match a large range of observed spectral properties, giving the number of "clouds" as a function of redshift, column density, spatial correlation length and perhaps linewidth all in good agreement with observations. Essentially, we are looking (at the low column density end of the spectrum) through relatively weak (barely nonlinear) gravitationally induced waves in the IGM. Matching computations to observations determines both the amplitude of the power spectrum at the relevant wavelength [Ref. #10] and also gives one information on  $\Omega_m$  [Ref. #11].

The X-ray clusters provide some important answers and some increasingly resistant puzzles. The rough number of clusters as a function of X-ray gas temperature and evolution of this function to moderate redshift seems to be in good agreement with the LCDM model quoted earlier [Ref. #12] and appears to argue strongly against  $\Omega_m = 1$  models. But in detail, we do not understand the X-ray profiles, which are less concentrated than straightforward simulations indicate should be the case [Ref. #13], and probably indicate the importance of additional physical input (*e.g.*, supernovae) not in the current simulations.

With regard to galaxy formation, there is better agreement and apparent understanding of the earliest phases [Ref. #14] (presumably because we have fewer observational constraints) than there is at low redshift where we, so to speak, know too much. It is not clear whether even the most gross features of galaxies (such as disk/bulge ratio) can be reliably determined by current codes [Ref. #15] with the most likely culprits being the absence of good methods to treat the multi-phase interstellar medium of normal galaxies.

An interesting and perhaps easier (since not such high spatial resolution is needed) problem to address is the question of "bias", defined as the ratio of galactic (stellar) density fluctuation to the underlying mass density fluctuations. Observations, [Ref. #16] semi-analytic calculations [Ref. #17] and hydro-simulations [Ref. #18, #19] agree that the amplitude of galaxy correlations is nearly constant with increasing redshift to redshift three, while the dark matter correlation amplitude decreases sharply (as expected from simple theory), thus indicating a rapid increase of "bias" with redshift.



A major part of this is due to Kaiser [Ref. #20] “peaks bias”. As galaxies were rarer in the past, the highest peaks were more strongly correlated than the more typical peaks. But, increasingly, the questions are being asked: “Was the problem properly formulated? Should galaxy formation be, in principle, only a function of dark matter density?” Within a galaxy, star formation surely is more vigorous in the higher density regions, but it also depends sensitively on temperature, with the coldest regions most fertile in producing new stars. Cosmologically, we know observationally the same is true: the very high-density, gas-rich clusters of galaxies are regions of especially *low* galaxy formation at redshift zero. Thus, as noted by Blanton *et al.* [Ref. #19], it would probably be best to think of bias as a function of density *and* temperature, increasing with  $\rho$  and decreasing with increasing T. Such a picture quite naturally explains the scale dependence of bias seen in several contexts.

Let me turn now to a subject which, I believe, has great “cosmological” promise – lensing, particularly the production of large angular scale features such as arcs. A statistical digression is useful here. If one tries to predict a typical property of the universe, the accuracy of the measurement will predict the accuracy of the test. Thus, measuring mass fluctuations on a  $10h^{-1}$  Mpc scale to a given precision fixes, *ipso facto*,  $\eta \equiv \sigma_8 \Omega^{0.6}$  to approximately the same precision. But, suppose one tries to predict the properties of the matter which, smoothing on a  $1h^{-1}$  Mpc scale, is over-dense by a factor of  $\geq 10^3$ . Only perhaps 5% of all matter is in this category and, due to the Gaussian nature of fluctuations, that percentage is exponentially sensitive to the value of  $\eta$ . Conversely,  $\eta$  is a logarithmic function of cluster abundance, and thus a tight constraint ( $\sim \pm 10\%$ ) on  $\eta$  is provided by a relatively poor measurement of the number density of rich clusters [Ref. #21, #22].

Now, of the rich clusters, only a small fraction (say 1/3) have a surface density above the critical level  $\Sigma = \text{const } cH/G$ , to produce multiple images. So, the matter in regions dense enough to provide arcs or large gravitational splittings is only 1%–2% of the total matter density. Thus, comparing the observed and computed number of large splittings provides an exquisitely sensitive test of models. Wambsganss *et al.* [Ref. #23] and Bartleman *et al.* [Ref. #24] have used this method to rule out certain models at a high confidence level. The method has great potential. However, as E.L. Turner (private communication) has pointed out, the sensitivity of the methods is a two-edged sword, easily capable of wounding the user: a 10% computational error in the predicted properties of these highly nonlinear structures can lead to an order of magnitude misestimate of the number of objects expected with a given set of properties.

### C) Some Summary Remarks with Regard to Cosmology

Perusal of symposia on cosmological topics over the past few decades quickly shows a dramatic transformation in intellectual style. From a concentration on the most gross geometrical features of the universe ( $H_0$ ,  $\Omega_0$ ,  $K$ ) and a self-consciously polemical tone normal to early phases of an intellectual activity,

the discussion has moved to what one might characterize as the “normal science” phase. Detailed observations at high, moderate and low redshift, with many parameters measured at about the  $\pm 10\%$  level, now severely constrain our imaginative flights of fancy. At the same time, there has been a realization that each model is mathematically precise (in a statistical sense), so it is no longer possible to have waffling discussions of the different possible outcomes of a specific scenario. Correspondingly, for more and more questions, very large scale numerical simulations can tell one the specific consequences of the models to the same  $\sim + 10\%$  level. One can say with certainty that there will be surprises ahead of us, but the confluence of rapidly improving observations, with computation becoming more realistic at a similar rate implies, that the lively cosmological debates of the future will be better informed than was possible in the entertaining past.

## 4 Concluding Remarks

There is a typical historical path followed for numerical studies of natural phenomena in astrophysics. All start in what I described as type (C) modelling, the simulation. Here, the scientist knows that the existing mathematical and physical picture is inadequate and is attempting to determine – varying both physical assumptions and mathematical/numerical techniques – the essential ingredients. This phase requires imagination, scientific judgement, carefulness in the avoidance of over-interpretation of success, and intellectual flexibility. Then, as time proceeds and the outline of the picture becomes clearer, the work proceeds towards either what I have termed type (A) or type (B) numerical modelling. In type (A), physical modelling, the improvements go towards a more accurate and comprehensive treatment of the physical processes. Examples of subfields in astrophysics for which this is relevant are stellar atmospheres and stellar interiors. While many important phenomena in these areas are still imperfectly understood, we know what is to be done in a methodological sense: more physical processes must be included in our treatments and the presently treated ones must be made more accurate (*e. g.*, more nuclear interactions, more precise cross-sections, rotation and turbulence treated more accurately in stellar interiors). Here, encyclopedic knowledge, patience and, again, carefulness are needed. In type (B) numerical modelling, greater mathematical prowess is required. The equations and physical processes are well understood, but the solutions are not. An example of a field where this applies is planetary dynamics. Both rigor and mathematical imagination are required.

While the computer cannot substitute for thought in any one of the three modes, it can be a great assist to pure thought, and, with the ongoing exponential growth in computer power, all three modes of numerical modelling are steadily gaining in importance to the field of astrophysics.

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