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Computational Astrophysics: The "New Astronomy" for the 21st Century

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Abstract. I discuss the role computer simulation has played in astronomical research, reviewing briefly the origins of the field only to place into perspective the enormous strides which have been achieved in recent decades. I will highlight areas where computational astrophysics has already made a scientific impact, and attempt to discover the conditions which lead to real progress. Finally, I will prognosticate on what the future may hold in store for the second "New Astronomy" revolution already well underway.

1. Historical Perspective

> *The "New Astronomy" ... seems assured of a most brilliant future.*
> G. E. Hale

Modern astrophysics as we know it began as a quiet revolution in the mid-19th century with the development of the science of spectroscopy by Kirchhoff, Fraunhofer and others. When combined with the revolutionary discoveries about the nature of matter provided by atomic and molecular physics in the first half of the twentieth century, astronomers suddenly had a new, powerful analytic tool to diagnose the cosmos—a tool in many ways more important to astrophysics than the telescope itself. For without spectroscopic measurements, astronomers would not have been able to detect the expanding universe, map the structure of our Milky Way galaxy, discover the quasars, or confirm the hot Big Bang origin of our universe. Indeed, spectroscopy underlies most of our twentieth century advances in astronomy.

Recognizing the potential of spectroscopy to transform astronomy into a quantitative *physical science*, solar physics pioneer and astrophysics founding father George Ellery Hale devoted his life's energies to realizing its potential. He called astrophysics the "New Astronomy" for the 20th century (Wright, 1966). In promoting this new way of doing astronomy, Hale made no small plans. Among his career accomplishments were the founding of the Yerkes, Mount Wilson, and Mount Palomar Observatories, the California Institute of Technology, the US National Academy of Sciences (NAS), and the Astrophysical Journal (Wright, 1966; Osterbrock, 1995).

In like fashion, digital computers have been quietly transforming astronomy and astrophysics since their invention in the mid-20th century. There is no doubt that computers are ubiquitous and indispensable tools for observer and theorist alike. In theoretical astrophysics, computer simulation allows us to probe additional dimensions of structure, dynamics and evolution for any astrophysical system including the universe as a whole (Norman, 1996). The breadth of topics presented at this meeting confirm this. In recognition of the growing importance of computers in astronomy, and especially theoretical astrophysics, the NAS Decade Survey of Astronomy and Astrophysics (the "Bahcall Report", Bahcall, 1991) devoted an entire chapter to it.

In my talk, I will focus on the role computer simulation has played in astronomical research, reviewing briefly the origins of the field only to place into perspective the enormous technical strides which have been achieved in recent decades. I will highlight areas where computational astrophysics has already made a scientific impact, and attempt to discover the conditions which lead to real progress. Finally, I will prognosticate on what the future may hold in store for the second "New Astronomy" revolution already well underway.

2. Early Pioneers

> *The immediate imitation in the laboratory, under experimental conditions subject to easy trial, of solar and stellar phenomena, not only tends to clear up obscure points, but prepares the way for developing along logical lines the train of reasoning started by the astronomical works.* G. E. Hale

While Hale was, of course, advocating what we now call laboratory astrophysics, he could just as well have been describing computational astrophysics. For computational astrophysics has become a theoretical laboratory for experimenting with astrophysical systems in much the same way laboratory astrophysicists experiment with astrophysical plasmas. While it is true the latter deals with reality and the former deals only with simulated realities, there are many similarities in goals and methodology. These include a concern about precision of measurement, the exploration of relevant parameter regimes, and the importance of qualifying the scope of validity of the results.

The view of the computer as a numerical laboratory took some time to emerge. Stellar evolutionists Martin Schwarzschild in the U.S. and Rudolph Kippenhahn in Germany were among the earliest pioneers to use digital computers to solve astrophysical problems. Both were at institutions where electronic computers were being designed and built shortly after WWII (Princeton and Gottingen). Both men made seminal contributions to stellar evolution theory in the 1950's and 1960's. The principal computational task in stellar evolution calculations is to solve the equations of stellar structure—four coupled ordinary differential equations—subject to certain boundary conditions and mass and composition constraints. In keeping with the parlance of the day, computers were viewed as numerical integrators—tools to evaluate a quadrature or compute a ballistic trajectory—rather than a tool for experimentation. The latter, more grandiose view of computers was held by the visionary John von Neumann. However, it is unclear whether his writings on the subject (Goldstine & von Neumann, 1963) reached the attention of the first computational astrophysicists.

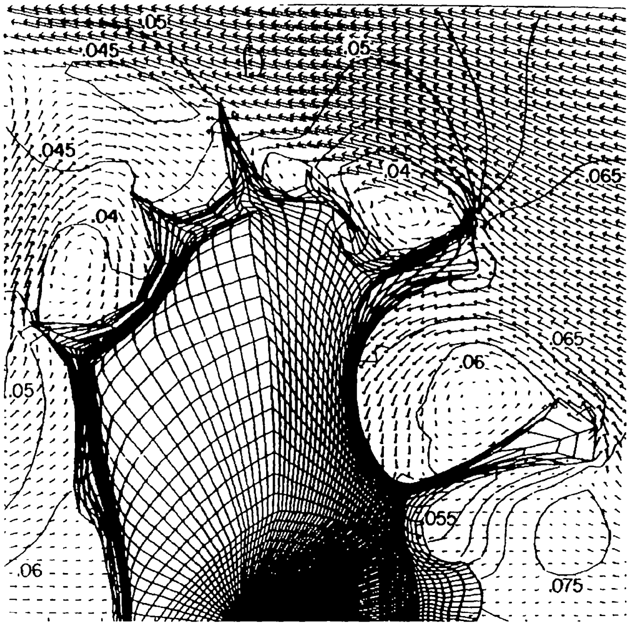

Figure 1. State-of-the-art numerical hydrodynamic simulation *ca.* 1975 of an interstellar cloud compressed by a passing interstellar shock wave. The two dimensional calculation utilized an innovative coupled Eulerian-Lagrangian grid of 28,000 cells and taxed the resources of a CDC 7600. From Woodward (1976), reproduced by permission.

The notion of computational astrophysics as experimental astronomy came about naturally when astrophysicists began to simulate dynamical systems in astronomy, principally stellar or hydrodynamical systems. These simulations are generally motivated by the question "What happens if?" more so than "What is the solution to these equations?". Remarkably, the earliest N-body experiment pre-dated digital computers by half a decade. Erik Holmberg simulated the tidal interaction of two galaxies with an analog computer consisting of an array of movable light bulbs and photocells each representing a point mass (Holmberg, 1941). Numerical integration was accomplished by placing the analog point masses on a mat inscribed with a Cartesian grid, and moving them about by hand according to the local gravitational acceleration determined by measuring the flux and direction of light incident on the stars' photocells (flux, like gravity, falls off as $1/r^2$). Each galaxy was represented by 37 point masses, arranged in circular rings.

Numerical stellar dynamics entered the modern era with the pioneering calculations of Aarseth, who in 1963 carried out the first N-body simulation of the dynamical evolution of a cluster of galaxies (Aarseth, 1963). Another pioneering effort was that of Juri and Alar Toomre, whose calculations of galactic encounters convincingly established a tidal origin for intergalactic tails and "antennae" in peculiar galaxies (Toomre & Toomre, 1972). While the Toomres' simulations assumed the test particle approximation, Aarseth's calculations were fully self-consistent, the force on each particle determined by direct summation over particle pairs. The success of these calculations launched a world-wide industry in gravitational N-body simulations as the tool of choice to study stellar, galactic

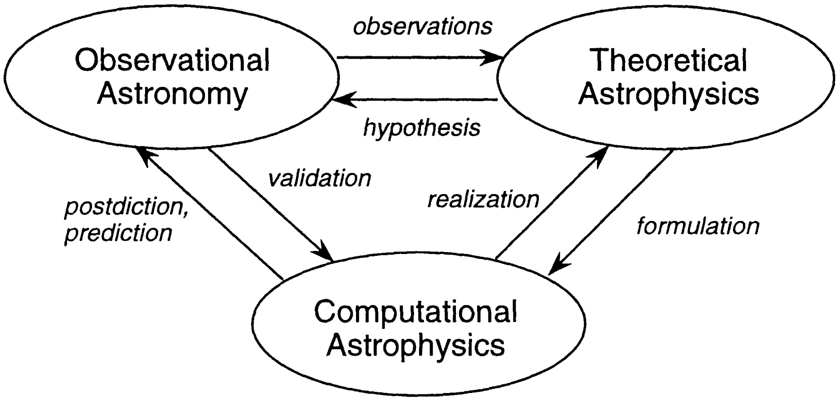

Figure 2. Synergies between observational, theoretical and computational astrophysics.

and more recently, cosmic dynamics. A good review of the early development in this field can be found in Aarseth & Lecar (1975).

Pioneers in astrophysical hydrodynamics employed computers in the late 1960's to simulate the birth and death of stars, and processes occurring in the interstellar medium. They include Richard Larson, who first self-consistently simulated star formation in 1-D spherical symmetry (Larson, 1969); W. David Arnett and independently James Wilson, who constructed the first detailed simulations of core collapse supernova explosions (Arnett, 1967; Wilson, 1971), rotating relativistic stars (Wilson, 1972), and hydromagnetically-driven winds (Wilson & LeBlanc, 1970); and Paul Woodward, who carried out the first multi-dimensional simulation of the implosion of an interstellar cloud by a shock wave (Woodward, 1976; *cf.*, Figure 1). Grids of several hundred points in 1-D, or several thousand in 2-D characterized these early simulations, in contrast to the millions used in today's large scale simulations.

3. Role of Computational Astrophysics

> *It is customary to distinguish sharply between observational and experimental sciences, including astronomy in the former. ... that distinction between these two methods of research is not so fundamental as it might appear.* G. E. Hale

Computational astrophysics interacts synergistically with observation and theory, and borrows elements from each, as illustrated in Figure 2. The interplay between observation and theory is standard and will not be belabored here. The interplay between computational astrophysics and the other two methodologies is perhaps less clear, and therefore I will discuss it briefly. Theory interacts with simulation in a number of essential ways. First, theory provides the mathematical formulation which is used in the construction of a numerical model, as well as defines the parameter space of solutions to be searched. Second, desirable analytic properties (*e.g.*, conservation laws) of the solution can be incorporated into improved numerical algorithms. Third, analytic solutions provide excellent test problems for code validation. In fact, it is often the case that failure to reproduce an analytic result stimulates the critical thinking required to invent more accurate algorithms. Finally, when analyzing the results of a numerical simulation, especially one involving many complex physical processes such as our examples, one attempts to construct simplifying analytic models which nonetheless capture the essential physics.

For their part, simulations provide realizations of theoretical models which are in general too complex to be solved analytically. These realizations are in essence the laboratory data upon which the correctness of theoretical models is tested. This is done in two ways. First, it is often the case in astrophysics that one is uncertain whether all of the relevant physics has been included. A failure of the simulation to reproduce the observed phenomena may indicate missing physics, bad numerics, bad observational data, or any combination thereof. Second, simulations build physical intuition by providing the modeler direct experience with the complex phenomena embodied in the governing equations. Improved physical intuition generally precedes the formulation of improved theoretical models.

Finally, the simulation must confront observations. Observations are the final validation of a model's correctness. In the early phases of model building, one strives merely to "postdict" the available observational data. As the quality of the data improves, models are either revised or rejected. A correct model will not only remain consistent as new observations accumulate, but will also predict and in fact suggest new observations to come.

4. Progress in Computational Astrophysics

Little progress can be made without powerful means.—G. E. Hale

Progress in computational astrophysics, as in other branches of computational science, has been paced by the development of and access to: (1) high-performance computer architectures, and (2) accurate and efficient algorithms. As shown in Figure 3, the peak speed of the fastest available supercomputer at any given time has advanced steadily since the ENIAC, the first fully electronic computer, was built 50 years ago. To a good approximation, speed has increased exponentially with time since WWII, with an e-folding time of about two years. This trend is expected to continue well into the next decade through continuing advances in VLSI circuitry and massively parallel architectures (Brenner, 1986).

Equally important has been the development and dissemination of robust, accurate and efficient algorithms for hydrodynamical and N-body simulations. Particularly influential have been, in hydrodynamics, the von Neumann and Richtmyer 1-D Lagrangian algorithm (Richtmyer & Morton, 1967); higher order-accurate Godunov algorithms for multidimensional gas dynamics (*e.g.*, Colella & Woodward, 1984); Smoothed Particle Hydrodynamics (Monaghan, 1992), the ZEUS codes for radiation magnetohydrodynamics (Stone & Norman, 1992b), and the Hawley, Smarr and Wilson algorithm for general relativistic hydrodynamics (Hawley *et al.*, 1984). On the N-body side, the following have received wide application: Aarseth's direct summation methods (Aarseth, 1971); the PM and P^3M algorithms of Hockney & Eastwood (1988), and the tree code of Barnes & Hut (1986) and Hernquist (1987). These algorithms, used separately

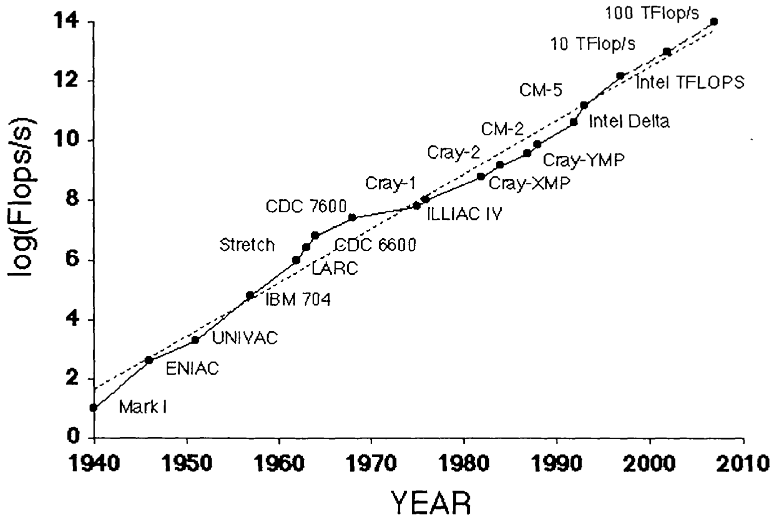

Figure 3. Growth in peak supercomputer performance *vs.* time (adapted from Kaufmann & Smarr, 1993). An exponential fit $2^{3t/5}$ is shown as the dotted line.

or in combination (*e.g.*, TREESPH, Hernquist & Katz, 1989), underly a large fraction of current computational astrophysics research.

Gains in algorithmic efficiency have roughly kept pace with hardware improvements. Consequently astrophysicists who have kept abreast of the latest algorithms and supercomputers have been able roughly to double the complexity of their simulations every year in recent decades. Until the mid 1980's, however, access to supercomputers was limited to a small cadre of researchers at defense laboratories or at a few well-endowed academic institutions. The establishment of the NSF Supercomputing Centers in 1985 opened up access to state-of-the-art supercomputers to the entire U.S. academic community. This development, as well as the subsequent creation of state and regional supercomputing centers, open supercomputing facilities at DOE and NASA labs, the emergence of powerful and affordable workstations, and the growth of the Internet have all played a role in increasing the number of computational astrophysicists roughly one hundred fold. As a result, computational astrophysics research has enjoyed a decade of unprecedented growth and progress.

The impact has been a broadening and a deepening of computational astrophysics research. As a result of improved hardware and algorithms, numerical simulations in the established areas of N-body and astrophysical fluid dynamics have matured in at least three significant ways. This is illustrated schematically in Figure 4, and by way of examples in Figures 5–7. Generally, there has been a progression from lower to higher dimensional simulations; from lower to higher resolution simulations; and from simple physical models to complex models embodying many physical processes. In any given field, progress tends to proceed along one axis at a time until a qualitatively new threshold of complexity and physical realism is reached. Research is carried out within the new paradigm, often community wide, until it is replaced by another advance, typically along an orthogonal axis.

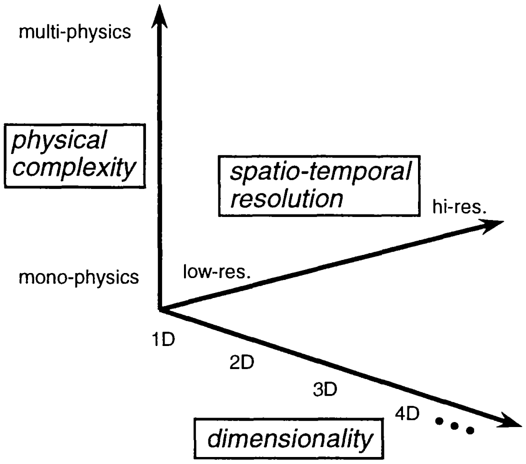

Figure 4. Progress in numerical modeling occurs along (at least) three axes in a conceptual phase space: dimensionality, spatio-temporal resolution, and physical complexity.

5. Case Study

Scores of problems suggest themselves for solution . . . G. E. Hale

To illustrate, consider simulations of a shock wave interacting with an interstellar cloud. This set piece problem has received considerable study over the years because it is a fixture in the McKee and Ostriker theory of the hot interstellar medium (McKee & Ostriker, 1977). A central question is how long the cloud survives after being hit by the shock wave. The earliest simulation carried out by Woodward (1976) correctly predicted the existence of Rayleigh-Taylor and Kelvin-Helmholtz fluid instabilities which grow on the cloud boundary and ultimately destroy the cloud. However, Lagrangian mesh tangling in the cloud interior terminated the calculation before cloud destruction was complete. The fully Eulerian calculations (MacLow *et al.*, 1994) shown in Figure 5 do not suffer from this defect. However, concerns about the effects of numerical resolution and assumed axisymmetry on the disruptive instabilities now come to the fore.

The steady improvements in supercomputers and algorithms in the 1980's permitted for the first time serious convergence studies to be made on multi-dimensional simulations. Convergence studies and their related validation test suites (see *e.g.*, Stone *et al.*, 1992) are now a standard part of good numerical methodology, and are an indication of a maturing field. The convergence study in Figure 5 illustrates that although the bulk deformation of the cloud can be captured with 50-100 cells per cloud radius, much higher resolution is required to capture smaller scale modes of instability which contribute to cloud disruption (Klein *et al.*, 1994).

The cloud is ultimately shredded by Kelvin-Helmholtz instabilities of the vortex sheet created by the interaction of the shock wave with the cloud's boundary. At the high Reynold's numbers of astrophysical fluids, the fully non-linear development of the K-H instability leads to turbulence, which is inherently 3-D. The first 3-D simulation of the shock-cloud interaction (Stone & Norman, 1992),

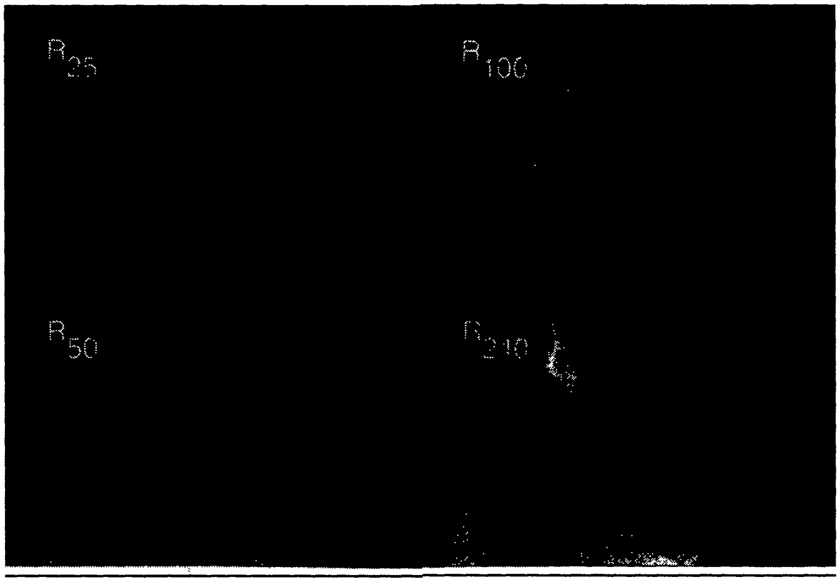

Figure 5. Convergence study of 2-D shock-cloud interaction simulations. The subscript in the figure label R_n refers to the number of cells used to resolve the initial cloud radius (from MacLow *et al.*, 1994)

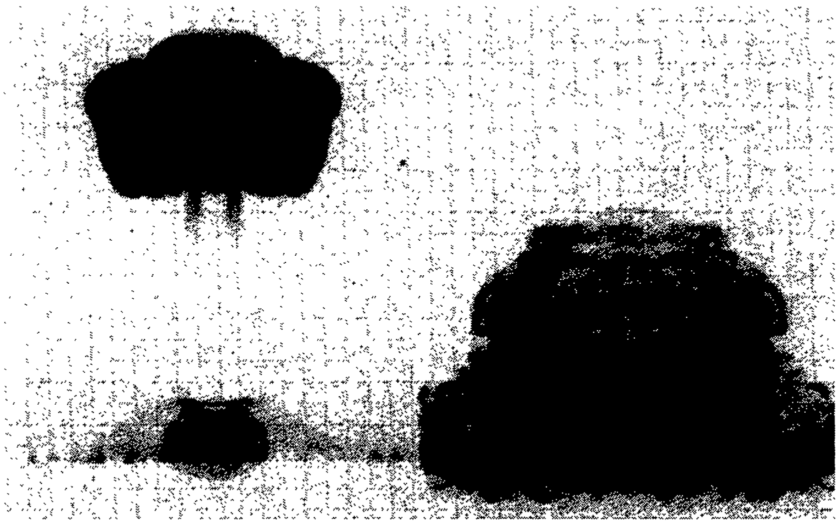

Figure 6. Two snapshots from a 3-D simulation of a shock-cloud interaction. Shown is the line-of-sight integrated fluid vorticity magnitude (from Stone & Norman, 1992a).

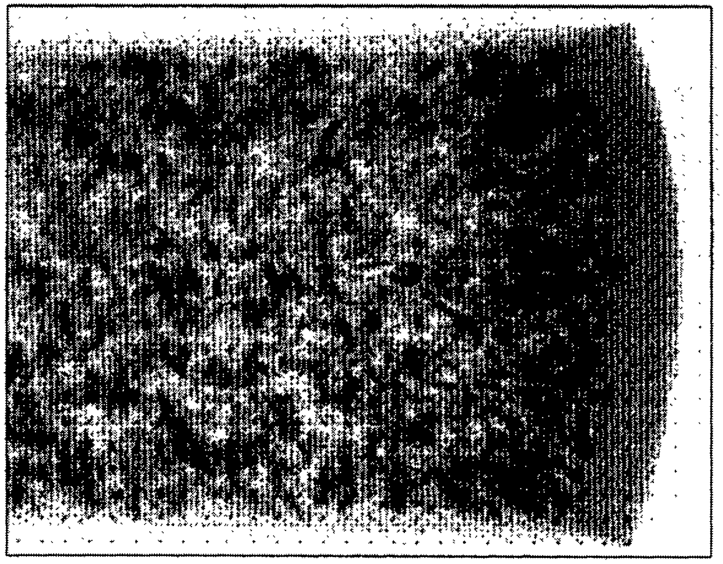

Figure 7. A numerical observation of a 3-D magnetic supernova remnant. Polarized radio surface brightness is shown in grey-scale, and polarization B-vectors are shown as vectors (from Jun & Norman, 1996)

shown in Figure 6, verifies this expectation, and provides the first realistic picture for the late phases of cloud disruption. Three-dimensional simulations such as these have only recently become practical with large memory parallel supercomputers. Although comprehensive 3-D convergence studies are barely feasible today because of computer limitations, isolated examples exist (Kang *et al.*, 1994; Jun *et al.*, 1995).

The simulations thus far have assumed ideal, adiabatic gas dynamics. Real interstellar clouds are magnetized, cool radiatively when shocked, *etc.* In order to engage observations in a meaningful way, simulations must also mature along the third axis of physical complexity. At the very least, additional physics describing the emissivity of the material must be added to the model so that observables can be computed, a step I call "numerical observations." Figure 7 shows an example of a numerical observation of a radio supernova remnant simulated by Byung-Il Jun and myself (Jun & Norman, 1996). A 3-D numerical MHD simulation of a young supernova remnant was carried out to compute self-consistently the complex structure of the magnetic field in the turbulent shell. The numerical observation is made by integrating the Stokes parameters along rays passing through the remnant, assuming radio synchrotron emission. The simulation reproduces the observed radial magnetic polarization in young supernova remnants, although the simulation is not predictive with regard to the radio luminosity since the relativistic electron population is not computed self-consistently. We have also not been able to converge on the amount of magnetic field amplification in the turbulent shell. Further model maturation is required to remove these defects.

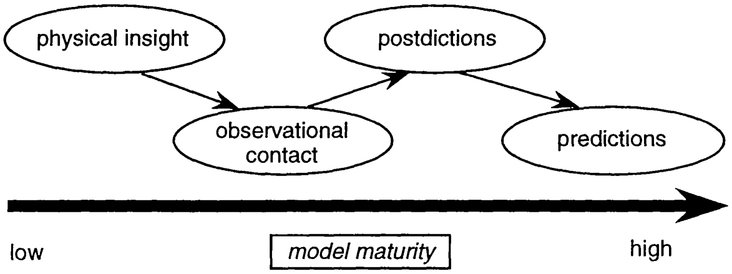

Figure 8. The primary contribution of a numerical model changes as it matures.

6. Scientific Impact

The scientific contribution of a numerical model changes as it matures. This is illustrated in Figure 8. In a few rare cases, such as the galaxy encounter simulations of the Toomres, an early, crude simulation will provide a key insight into the nature of an astrophysical phenomenon. A recent example is the still somewhat controversial role of neutrino-driven convection in core collapse supernova explosions (Norman, 1996). Such simulations change the way we think about things, and constitute important scientific contributions in their own right. Often, these simulations can be reduced to a cartoon or a mathematical toy model *post facto*, and become enshrined in elementary astronomy textbooks.

More often than not, early models miss essential physics inherent in a phenomenon, or are of insufficient resolution to simulate it accurately. Such models require substantial maturation before observations are engaged in any meaningful way. However, once all the physics is included and computers are adequate to the task, rapid progress generally follows. Stellar evolution theory is the premier example of this. The equations of stellar structure were known in the 1930's, the missing piece of physics—nuclear energy generation—was supplied in the 1940's, serviceable opacities and numerical algorithms were in place by the end of the 1950's, and adequate computer power was available in the 1960's. Scientific progress swiftly followed. An important factor for progress was the abundant, high-quality observational stellar data exhibiting clear statistical trends. Stellar evolution calculations first rationalized these data into a coherent theory, and then proceeded to make testable predictions. Frontier areas remain in stellar evolution theory. However, these invariably involve dynamical phenomena (*e.g.*, star formation), three-dimensional physics (*e.g.*, convection, symbiotic binary stars), or other complications, which up the computational ante.

Reflecting on other areas of computational astrophysics which have made a definite scientific impact, I find the following conditions must be met: (1) complete physical model; (2) good numerical algorithms; (3) adequate computing power; (4) unambiguous observational data; (5) insensitivity to initial conditions where they are unknown, *or*, sensitivity to initial conditions where they are known (or at least knowable). When these conditions are met, simulations have predictive power and are able to rationalize observations into a proper theory. Areas where this is occurring include dynamic stages of stellar evolution, stellar and galactic dynamics, galaxy interactions, and cosmological structure formation. Rapidly maturing areas include accretion disks, jets and outflows from young stars, morphology of planetary nebulae, Type Ia and Type II supernova mechanisms, accretion onto compact objects, galaxy formation and evolution, and the structure of the Lyman α forest. Areas which still lack one or more of these criteria include, in my opinion, star formation, structure of the interstellar medium, active galactic nuclei, astrophysical dynamos, turbulent convection in stars, astrophysical particle acceleration, and radio galaxies.

7. Future Outlook

> *Questions of all degrees of complexity remain to be answered, and every day sees their number increased.* G. E. Hale

Supercomputing hardware performance is expected to continue improving at its historical rate, with computing speed doubling roughly every 20 months, for at least the next decade. Supercomputers with peak speeds in excess of a teraflop (10^{12} Flop/s) will be operational at the Department of Energy weapons labs by 1998. Ten years after that we can expect to have 100 teraflops. My own center, the NCSA, will have a teraflop computer available to academic researchers by the turn of the century. This guarantees that computational astrophysics will continue to develop and mature. Teraflop supercomputers will permit models of realistic complexity to be simulated in 3-D at high resolution (*e.g.*, $1{,}024^3$.) This kind of computer power will benefit, in particular, research in cosmological structure formation, stellar convection, star formation, supernova phenomena, and the relativistic dynamics of coalescing binary neutron stars and black holes.

However, recent history has shown that more significant than supercomputers to the spread of computational astrophysics research are affordable workstations and PCs. These computers follow the same speedup trend, but lag supercomputer performance by about 10 years. For example, by the year 2000, affordable workstations with 1 gigaflop/s processors and 1 gigabyte of RAM will be on the market. This means that the average university astronomer will have the equivalent power of a Cray-2 supercomputer on their desktop. What will this machine be used for, and where will the software come from?

Since 1993, the Laboratory for Computational Astrophysics (LCA) which I direct has developed and distributed astrophysics simulation software to the international research community (visit our web site: `lca.ncsa.uiuc.edu`.) Two programs for astrophysical fluid dynamics called ZEUS-2D and ZEUS-3D, developed by Jim Stone, David Clarke and myself, have attracted a large following. Curiously, most users prefer to install the software on their local workstations rather than use a supercomputer. This limits the size and sophistication of the calculations they can do. However, with gigaflop workstations just around the corner, that will change. High-resolution 2-D simulations and medium-resolution 3-D simulations will be routinely doable on desktop machines. Moreover, with the emergence of the Web as a metaphor for information access and the coming of higher network bandwidths, we can envision an era of high-end web computing where the users' PC becomes an interface to a simulation running on a remote supercomputer. Work has begun on a web-based LCA computational workbench to make this idea a reality.

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Part I

SOLAR SYSTEM DYNAMICS