1a) Project Title Astrophysical Hydrodynamics in Three Dimensions

1b) Project Acronym Astrohydro3D

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2a) Summary The genesis, structure and evolution of astrophysical objects has one common denominator: *continuum mechanics*. Since practically all cosmic matter is gaseous, this boils down to *hydrodynamics*. Numerical hydrodynamics in astrophysics is in the process of breaking through two barriers: first, the inclusion of the realistic treatment of many more physical processes, in particular multi-fluid interaction and radiative transfer ('large scope'); second, the extension to fully three-dimensional flow ('large scale'). The techniques for coping with these aspects have become so far-reaching and so specialized, that it is no longer feasible to build and implement them all locally. There exist many techniques, such as adaptive mesh refinement (AMR), that we could use. This proposal aims at bringing the latest algorithmic, numerical and computer-hardware techniques to the field of astrophysical hydrodynamics in the Netherlands. Our group is working on cosmological applications, relativistic flow, radiation hydrodynamics, cooling accretion flows, chemically reactive and dust-driven flows, stellar evolution, nucleosynthesis and supernovae. This proposal aims at the co-ordination and reinforcement of these efforts.

2b) Purpose Our *mission* is to understand things. Our *goal* is to understand how things formed in the Universe. Our *strategy* is the application of known physics as it is dictated by the observations of the objects whose origin and evolution we wish to comprehend, using and creating advanced computer techniques. Our *tactics* are to proceed from our firm base of two-dimensional numerical hydrodynamics, using open-source computer methods wherever feasible, implementing the targeted physical processes in sequence, proceeding to increasingly geometrically complex situations. Our *products* are improved understanding, predictions and suggestions for future observations, and better computational techniques.

3) A&A/NWO Classification (02.08.1) Hydrodynamics - (02.18.7) Radiative Transfer - (02.19.1) Shock Waves - (08.13.2) Stars: mass loss - (08.23.3) Stars: winds, outflows - (09.16.1) Planetary Nebulae - (08.19.4) Supernovae - (11.06.1) Galaxies: formation - (12.12.1) Cosmology: large-scale structure of the Universe - (1.1) Parallel systems - (5.4) Parallel algorithms

4) Composition of the Research Group

Staff Member	Title	Specialization	hrs	Institute(s)
Icke, Vincent	prof.dr	astrophysics	16	Sterrewacht Leiden
				& Pannekoek Instituut

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Mellema, Garrelt		dr	radiati dynam	ion hydro- nics	24	KNAW Research Fellow at Sterrewacht Leiden
Simis, Yvonne		drs	•	dynamics ting flows	36	graduate student at Sterrewacht Leiden
Van de Weygaert, R	ien	dr	cosmo	0	16	Kapteyn Instituut
Langer, Norbert		prof.dr	astrop	hysics	8	Sterrenkundig Instituut at Utrecht
Deul, Erik		dr	compu	ter science	e 8	Sterrewacht Leiden
To be appointed	Sup	oerviso	r	Institute	е	Subject
Graduate student Graduate student Graduate student	Lang	lema/Icl ger de Wey		Leiden Utrecht Groninge	n	mass loss of low mass stars mass loss of high-mass stars large-scale structure formation

5) Research School All astronomy research in the Netherlands is co-ordinated by NOVA, the Netherlands Research School for Astronomy.

6) Description of Proposed Research

6A) What Are We Doing Now? In what follows we will describe the *status quo* at Leiden, Groningen and Utrecht, and in (6B) indicate how our work will be promoted by this proposal. Currently, steps are being undertaken to start new research on advection-dominated accretion flows and gamma ray bursts at Amsterdam (in collaboration with Spruit and Dullemond at Munich) that would also benefit from our initiative.

The following physical aspects have received attention in association with our group: cosmological applications (Icke, Van de Weygaert); relativistic flow (Eulderink, Mellema); radiation hydrodynamics (Mellema); chemically reactive and dust-driven flows (Simis, Icke); stellar evolution, nucleosynthesis and supernovae (Langer). The current proposal aims at the co-ordination and reinforcement of these efforts, supported by new computer technology implemented at Leiden by Deul.

Stellar death Our research in this area focuses on the formation of circumstellar envelopes. This presents an interesting, subtle and complicated interplay between stellar evolution, hydrodynamics, chemistry, dust formation, and radiative transfer. Substantial improvement in the quality of the observational data has motivated the modelling of molecular line and dust grain emission from the stellar winds. The conditions are often far from thermal equilibrium. In most cases the radiative transfer is at least partly optically thin, and therefore non-local. The geometries can be quite complicated and *in realistic cases are invariably three-dimensional*. This strongly motivates a substantial increase in the number of physical mechanisms included, in the subtlety of algorithms, and in computer power.

The understanding of main-sequence stars is one of the triumphs of astrophysics. However, massive stars (always) and low-mass stars (near the end of their lives) lose matter from their surface at such a rate that the classical models must be seriously altered. Unfortunately, this mass loss rate cannot yet be calculated from first principles, and hence has to be estimated using observational data and approximate numerical models.

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The origin of shell structures around planetary nebulae and around stars in the phase beyond the asymptotic giant branch (AGB) post-AGB has long been a mystery. Our calculations of dust-driven winds show the formation of such shells (Fig.1), closely resembling the observations in spacing, time scales, and density amplitude. The shells are formed as a consequence of the strong coupling of various physical processes (e.g. grain formation and growth, hydrodynamics and gas chemistry). Also the tendency of solid grains to drift with respect to the gaseous matter turns out to be crucial.

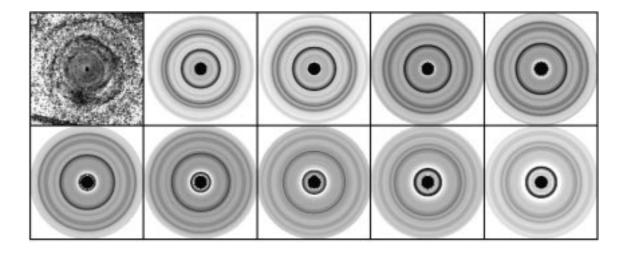


Fig.1 Upper left frame: Composite B+V image of the shells around IRC +10216, with an average radial profile subtracted to enhance the contrast (adapted from Mauron & Huggins, 1999). Other frames: series of snapshots from our numerical hydrodynamics code. Plotted is the dust column density, also with an average radial profile subtracted. The average radial profiles are calculated for each snaphot separately, hence the slight difference in color from plot to plot. The theoretical profiles are shown for ages 44, 81, 118, 164, 211, 252, 295 and 342 years with respect to the first frame. The size of the computational grid corresponds with the field of view of the observational image (131" x 131") and a distance of 120 pc.

Ultimately, stars lose so much mass that they expose their cores, which emit ionizing radiation that blasts into the material previously lost by the star. Ionized gas is easily observed at optical wavelengths, providing another way to study the effects of mass loss on the evolution of stars. These bright optical nebulae are known as *planetary nebulae*. Most of them have non-spherical shapes (Fig.2). The elucidation of the mechanisms behind this non-spherical hydrodynamical behaviour is one of the main successes of our group (in conjunction with Balick at Seattle and Frank at Rochester). Even though our work on bipolar nebulae has become 'industry standard', we are determined to extend our research from two to three dimensions.

Combining hydrodynamics with radiative transfer calculations is next to the transition to 3D calculations, the other logical step in the development of hydrodynamic modelling. In many applications the role of the photons is essential and always the radiation is what we finally observe. The work of Mellema (Fig.3), together with various

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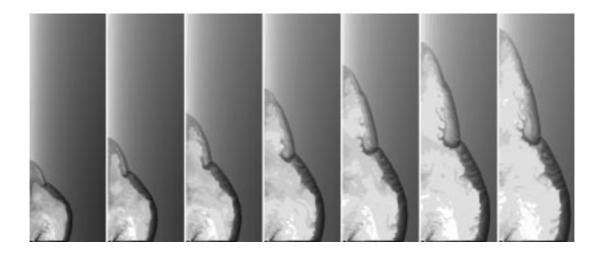


Fig.2 Evolution of the density field (log scale) of a bipolar nebula. Each image is cylindrically symmetric about the left edge, and reflection symmetric about the bottom edge. The simulation shows the formation of polar protrusions, which are tentatively identified with the *ansae* observed in some bipolar nebulae.

collaborators, such as Frank, Raga, Lundqvist, has broken new ground in this area, but (as in the case with 3D calculations) further progress needs the use of AMR methods and parallelization in order to be able to use the modern supercomputers.

The most massive stars suffer the most violent endings. Explosions of the sort that have occurred in Eta Carinae (Fig.4) and in SN1987A have demonstrated that here, too, the interaction with the stellar envelope is a very complex and intriguing phenomenon. The shaping of such nebulae is analogous to the processes occurring in bipolar planetary nebulae, but in these cases particle acceleration, nucleosynthesis, and other high-energy processes must be taken into account. Our findings indicate that the dense cores of such massive stars are convectively unstable during the final seconds of the onset of the explosion, leading to enormous density gradients and chemical inhomogeneities.

The largest cosmic structures The question of why, how and when galaxies evolved from the barren early Universe remains at the forefront of astrophysics. Observational supertools like the VLT and Keck telescopes and the Hubble Space Telescope have given us an unprecedented view of the conditions and objects populating the Universe down to a fraction of its present age.

These observations are yet to be matched by theory. One of the major reasons for this deficiency is that the development of galaxies is not governed by purely gravitational forces. On the contrary, galaxy formation is likely to be a complex feedback process in which gravity (Fig.5), radiative transfer, star formation and stellar death are involved. The chief intermediary agent in this interplay is probably radiation.

So far, the vast majority of galaxy formation computations has relied on smoothedparticle hydrodynamics (SPH). The word 'hydrodynamics' in this acronym is an overstatement: from the hydro point of view, SPH has immense deficiencies, its intrinsically 3D character notwithstanding. In particular, SPH is a first-order method, not suitable for the tracing of shock waves, and it is severely limited by shot noise effects. We are among those who think that 3D hydro continuum methods must replace SPH. Classical

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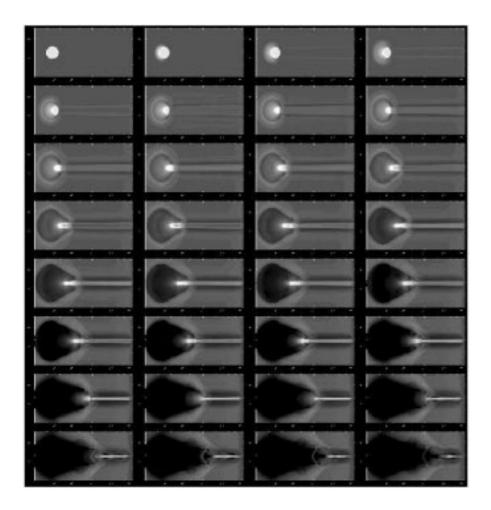


Fig.3 The photo-evaporation by radiative ionization of a dense knot. After a shock has moved through the knot it starts to accelerate (Oort-Spitzer rocket effect). The region behind the knot starts to recombine and cool, and accretes material forming a dense tail. In the final frame the original knot has completely evaporated and only the tail remains.

fixed-mesh methods will not suffice, due to the 3D character of the flows and due to the vast range of mass and length scales involved. One is forced to consider physically small and extremely dense regions on an equal footing with tenuous regions that span immense volumes.

6B) What Will We Do Under This Proposal?

Overall aim and motivation This proposal is meant as a collaboration, bringing together our expertise on physics- and computer-intensive hydrodynamics. Numerical hydrodynamics in astrophysics is in the process of breaking through two barriers: first, the inclusion of the realistic treatment of many more physical processes, in particular multi-fluid interaction and radiative transfer ('large scope'); second, the extension to fully three-dimensional flow ('large scale'). This proposal explicitly aims at progress on both of these fronts, building on our own expertise and on open-source methods developed elsewhere. For an excellent overview over what can be done, see the contributions by Dorfi, LeVeque, Mihalas and Müller (LeVeque et al., 1998).

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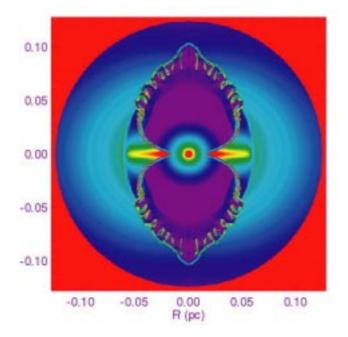


Fig.4 Snapshot of the evolution of Eta Carinae: circumstellar density due to three consecutive winds (fast, slow, fast), assuming the slow wind comes from the star close to critical rotation and being strongly concentrated to the equatorial plane.

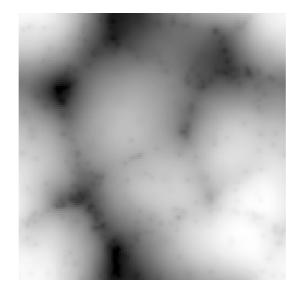


Fig.5 Simulation of the potential field in a universe that is fragmenting in the form of a Voronoi tessellation. The image spans two minutes of arc in the sky.

We aim at a quantum leap in astrophysical hydrodynamics: three dimensions, high spatial resolution, and as much detailed physics as possible. Essential ingredients for this are mesh refinement techniques and parallelization. This provides the common ground for our various researches, and we will maintain an open and constant exchange of our techniques and solutions. We are prepared to publish our methods as open-source code under the usual GNU licensing terms.

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The only extant tool for tackling these problems is adaptive mesh refinement (AMR; e.g. LeVeque et al. 1998). We are exploring the possibility of connecting AMR schemes with our proven methods for subdividing spatial volumes, such as the Voronoi tessellation and the Delaunay triangulation. Awaiting their implementation in AMR computations, we have focused on idealized circumstances in an attempt to isolate gravitational processes that are likely to be relevant in the formation of smaller-scale objects. We are investigating the possibilities of AMR-techniques based on the Delaunay-Voronoi triangulation (Fig.6), a partitioning of space that has a large number of superior mathematical properties.

7) Work Programme The staff members listed above are already working on research related to this project. The graduate student appointments may be spread out over two years, starting in autumn 2001 and running for four years each. In the first year, all effort will be directed towards the conversion of our current techniques to three dimensions. These will be tested and benchmarked on our Beowulf-system. Parallel proposals for large scale work on the national Teras-machine will be written, and submitted to NCF. In the second year, contingent on the granting of computer time, we will enter a stage in which the newly appointed graduate students will begin with the exploration of our new methods and initial production work. The next two years are obviously more difficult to foresee, but under normal circumstances these should contain the main production period. Publications will be written as progress reports.

The various parts of our programme will be carried out simultaneously, so there is no single-stranded time-line. Mellema has started his KNAW research project in the Leiden Theory Group. Simis is in the final phases of her Ph.D. Thesis, thus allowing for an extension of her current work to two and three dimensions. Icke's analysis of the kinetic theory of strongly non-equilibrium dust/gas mixtures will be wrapped up by then, and he expects to concentrate on the implementation of AMR techniques in the 2000/2002 season. Van de Weygaert will have his cosmological computations adapted for the purpose of this project by mid-2001.

Deul's ongoing experiments with the Beowulf system now have reached the stage where an actual machine has been built. It is already being used by Mellema. Testing and implementing the software should be finished by mid-2001. Extension to the needs of this collaboration is straightforward, as is the building of clones in other institutes.

8) Expected Use of Instrumentation The type of studies proposed can only be done with high capacity computer equipment, i.e. with a parallel computer. In order to keep a high standard in both theoretical and observational astrophysics, we need to continually upgrade our computer resources in conjunction with our numerical methods. Recent developments in parallel computing protocols (the *Beowulf* system) are being actively pursued at Leiden. This allows the use of commodity components (such as individual small machines) as nodes in a parallel configuration. This approach is both efficient and flexible, i.e. the nodes can be used as single computers, or as one 'virtual' machine. Hydrodynamical computations on such a system are almost 'trivially parallelizable'.

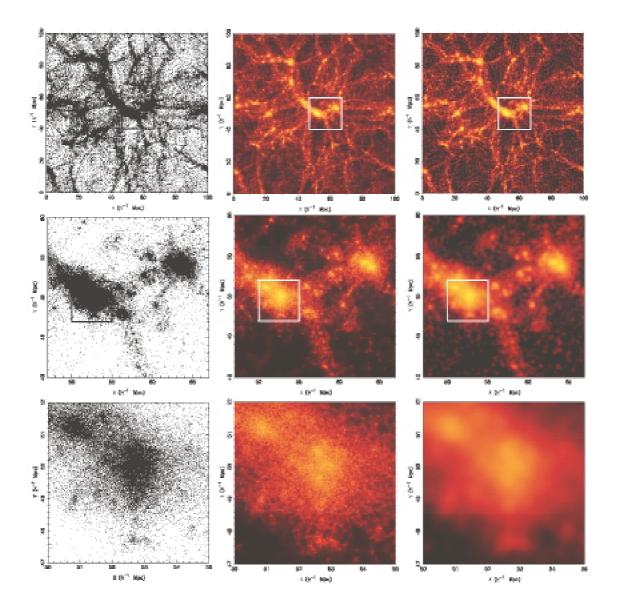


Fig.6 Comparison of the performance of the Delaunay density estimating technique with a conventional grid-based TSC method in analyzing a cosmological N-body simulation. Left column: the particle distribution in a $10h^{-1}$ Mpc wide central slice through the simulation box. Central column: the corresponding Delaunay density field reconstruction. Right column: the TSC rendered density field reconstruction. Logarithmic scale of the density fields runs from $\delta\rho/\rho = 0$ to 2400.

Expected Use of Observations While our proposal is plainly theoretical, we will always gear our efforts towards the understanding of actual phenomena. In this sense, our work will have a clear 'third way' aspect of computational modelling. We believe to have been quite successful at this in the past, and expect to do better still within the framework of this proposal. Astrophysics is in a very rapid phase of development, both in terms of the observational equipment and the possibility to do theoretical modelling. Observationally, a large number of unique facilities have become, or will soon be, available. This includes the HST (Hubble Space Telescope) and the ESO VLT (Very Large

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Telescope) in the optical, ISO (Infrared Space Observatory) in the infrared, AXAF (Advanced X-ray Astrophysics Facility) and XMM (X-ray Multi-mirror Mission) in the X-ray, and SEST (Swedish-ESO Submillimetre Telescope) and LSA (Large Southern Array) in the radio.

9) Requested Budget At current listings, the expenditure for a graduate student is DFL 50,000 p/a. We request three graduate studentships (four years each), and adding to this the DFL 7350 personal discretionary money, plus DFL 6000 institutional bench fees, brings the proposed personnel cost to DFL 640,050. The material budget of DFL 50,000 will be used for setting up a 20-processor *Beowulf* system, to be used as a test bed for the large scale computation runs. Thus, the total requested budget is DFL 690,050.

10) References The following is a very abbreviated list of key publications relating to the scientific aspects of the above proposal. More detailed technical information on the proposed computer setup is available on request.

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