

DISSERTATIONES ASTRONOMIAE UNIVERSITATIS TARTUENSIS 7

SIMULATION OF THE EVOLUTION OF LARGE SCALE STRUCTURE ELEMENTS WITH ADAPTIVE MULTIGRID METHOD

IVAR SUISALU

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List of Publications

- I A. L. Melott, J. Einasto, E. Saar, I. Suisalu, A. A. Klypin, S. F. Shandarin, 1983. Cluster analysis of the nonlinear evolution of large-scale structure in an axion/gravitino/photino- dominated universe. Phys. Rev. Lett. 51, 935.
- II I. Suisalu, 1987. Multigrid versus FFT methods for simulating gravitational gravitational collapse. Preprint Tartu Astrophys. Obs. A-1.
- III I. Suisalu, 1988. Theory of Lagrangian singularities and standard initial velocity fields ((*in Russian*). Publ. Tartu Astrophys. Obs. 52, 98.
- IV T. Schramm, I. Suisalu, L. Nieser, 1991. N-Body techniques for microlensing. In: Gravitational Lenses, Lecture Notes in Physics No. 406, Springer-Verlag, 383.
- V I. Suisalu, E. Saar, 1995. An adaptive multigrid solver for highresolution cosmological simulations. Mon. Not. Royal Astr. Soc. 274, 287
- VI I. Suisalu, E. Saar, 1995. Gravitational collisions in cosmological Nbody codes. (submitted to Mon. Not. Royal Astr. Soc.).

Introduction

Modelling of the evolution of the large-scale structure of the Universe is a well established method to test predictions of cosmological theories against observations. The status of the current theories and that of the observational material has raised the need for new approaches and methods of numerical simulations.

Until now the astrophysical community has used two types of codes for modelling gravitational problems. The first codes assume that systems consist of pointlike particles and they find force by direct summation over particles or their complexes. These codes are called tree-codes and their computational cost scales as $O(n \log(n))$, where n is the number of massive points.

The second class of codes assumes a continuous matter distribution and uses spatial grids to describe it. Among the grid methods for solving gravitational field equations the Particle-Mesh (PM) and the P³M (Particle-Particle-Particle-Mesh) codes are the best known. Both of them are based on the Fast Fourier transform (FFT) for which the computational cost scales as $O(n_g \log(n_g))$ (n_g is the number of grid points) and they are restricted to homogeneous grids. The spatial resolution of the last method (P³M) is enhanced by direct summation of forces between nearest neighbours, which means that essentially it is a particle method belonging to the first class of codes.

Both the P^3M code and the tree-code are based on the paradigm of individual clouds of matter. Although a softened force is usually used, it is not clear how well the massive clouds represent the essentially continuous distribution of dark matter. It is still not verified how collisionless these quasi-direct force summation methods are. In principle, grid based methods that do not treat matter explicitly as a collection of discrete massive particles, should be more appropriate for dynamical simulations of the evolution of the distribution of dark matter in the Universe.

An alternative way to the Fast Fourier Transform methods of solving the field equations is to use multigrid methods for partial differential equations. In essence these are iterative algorithms which are accelerated by the use of many hierarchically organized subgrids, and their computational cost scales as $O(n_g)$. The main advantage of these methods is the ability to work with grids of arbitrary size and discretization types. Using adaptive MG-algorithms one can generate local grid refinements automatically during the solution process. So one can adapt the spatial resolution of the solution in regions of interest and to obtain the result in a more optimal way.

Cosmological simulations are very complex due to a large range of scales which should be resolved in order to get reliable answers to our questions. The largest length-scales in space which define the computational domain are about several hundreds of Megaparsecs (Mpc) and the smallest scale which should be resolved is the size of the galaxy being typically about 10kpc. This gives for the minimum number of gridpoints in one coordinate direction around 10⁴ in case of an uniformly spaced grid. In 3-D we shall need accordingly 10¹² gridpoints. To resolve an initially essentially continuous matter distribution one needs at least 10 masspoints for a grid cell (in order to reduce the Poisson sampling noise), which gives an estimate of 10¹³ masspoints to be used for large-scale dynamics. Of course this can not be accomplished even with the most powerful present day supercomputers, so it is necessary to resort to more sophisticated adaptive grid methods. The ability of multigrid methods to deal with such multiscale problems

The ability of multigrid methods to deal with such multiscale problems gives us hope that they may be valuable in all problems of computational cosmology, but especially in simulations of clusters and superclusters of galaxies. This is not only because of the ability of the code to use adaptive resolution, but also because of the flexibility in incorporating the influence of the surrounding mass distribution. Until now the only boundary conditions used have been either periodical boundary conditions for the PM and P^3M or vacuum boundaries for the tree-code (with an added quadrupole tidal field in some cases, or approximate periodical forces). These boundary conditions force one to select non-generic patches of the Universe to model, with the only justification that these are the initial conditions our simulation codes can handle. Multigrid methods, in contrary, can efficiently handle any type of boundary conditions.

There are several problems of astrophysical interest which are very demanding in a computational sense, where multigrid methods could be useful.

The first two computational problems belong to the category of the evolution of the large-scale structure in the Universe. The evolution of initially smooth perturbations in a cold self-gravitating medium gives rise to the formation of singularities in the distribution of density as described by the theory of Lagrangian singularities. This theory states that there is a fixed number of stable singularity types. This theory is essentially scale free and applies to general matter flows (of potential type), but as the theory is local in space-time, which means it is quasi-linear, one can use this theory on scales comparable with superclusters of galaxies. The problem here is what is the real non-linear fate of these density singularities. Using the theory of Lagrangian singularities one can construct generic initial velocity fields for different types of singularities and then use these initial conditions for dynamical simulations. The result of this work together with a recipe for galaxy identification could give us an idea how the dark matter component of the Universe forms the elements of the large scale structure.

Another computationally intensive problem of cosmology is the simulation of galaxy clusters, where the large density range arises naturally. Identification and classification of simulated clusters depends heavily on the ability of the code to treat the substructure of high density regions and to approximate galaxy formation. There are still methodological problems about the role of the two-body relaxation in those simulations and how the large scale gravitational environment influences the clustering of galaxies.

Another field of gravitational astrophysics which needs special efforts in computational sense is gravitational lensing. The deflection field of a gravitational lens is proportional to the two-dimensional force field produced by the projected mass distribution which bends the light of background sources. For complicated matter distributions, as needed, e.g., for the simulation of the microlensing effect, it is necessary to invoke fast Poisson equation solvers as given by the multigrid approach. The idea is that the caustic pattern produced by the stars in a lensing galaxy can cause the lensed sources (such as quasars) to change their brightness on timescales from days to decades. The analysis of the observations of this effect could give important information on the content of clumpy matter (stars, brown dwarfs, black holes etc.) in galaxies. First estimates show that this method is sensitive to objects down to $10^{-7}M_{\odot}$ but simulations with more stars (10^6) are needed. The first simulations of lightcurves with 10^5 stars show the efficiency of the adaptive multigrid method for this particular problem. We have described the work done on simulating microlensed lightcurves in paper IV, but as this is only a summary of the conference report, I did not include it in the present thesis.

The dissertation presented here is a collection of articles showing the history of the development and application of the adaptive multigrid method in cosmological simulations.

The first chapter (paper I) describes the results of the analysis of the evolution of the large-scale structure for a particular type of the dark matter. This paper was written long ago and was one of the first to introduce a new type of dark matter – the cold dark matter (CDM) that serves as a standard dark matter model for the Universe today. It uses the same methods of comparison of simulation results to observations as used until now and touches the theoretical problems which are actual today also. It is also the first paper where cluster analysis was applied to the analysis of simulations. Straightforward cluster analysis algorithms scale as $O(N^2)$, where N is the number of particles, and could not be used; in this paper a much faster algorithm, based on division of space into ordered beams, is developed and used. In total, this chapter gives a quite comprehensive overview of problems of numerical simulations of the large-scale structure of the Universe that are mostly still unresolved.

The second chapter (a translation of paper III that was originally published in Russian) builds the basis for the theory of formation of superclusters of galaxies. Innovative here is the direct derivation of initial velocity fields for the typical geometry of the structures forming in dark matter, using the theory of Lagrangian singularities. In this chapter there is given a quite elaborate overview of the theory and the derivation of standard initial velocity fields which should exist in generic motion of matter under gravitation. These initial velocity fields serve as a basis for a future detailed modelling of superclusters using an adaptive multigrid approach. At the moment there are yet not enough observational data collected to describe the huge superclusters in sufficient detail to warrant building of detailed models, but with the huge volumes of new data planned to come from the new galaxy redshift surveys in progress, the results of this chapter should be put to use soon.

In the third chapter (paper II) multigrid methods for simulating the evolution of self-gravitating structures are introduced. It is a pilot work meant to compare two competitive methods of solving Poisson equation: one based on the Fast Fourier Transform (FFT) that is the most popular algorithm used presently, and the second is the multigrid version. The results show that the last method is quite comparable to the FFT as far as computer resources are considered (memory requirements, speed etc.) and from the physical point of view, the multigrid algorithm seems to be better in simulating the collapse of an isolated one-dimensional sphere (the example is chosen as one of the few exact solutions of gravitational dynamics known).

The fourth chapter (paper V) introduces the full three-dimensional adaptive multigrid code written by the author (this is the main result of the dissertation) and decribes its tests for cosmological problems. As an application the birth of a pancake-like structure (as the simplest singularity, it should describe the most common geometry of a structure element) is simulated using the initial velocity field derived in Chapter 2. This chapter shows the high-resolution properties of the adaptive multigrid method. We have achieved here the first time a (linear) resolution of L/1024, where L is the size of simulation cube, using only a workstation. Such resolutions have

not yet been achieved even on supercomputers; our trick is that the adaptive multigrid selects high resolution where it is needed, not everywhere over the full simulation volume.

In the fifth chapter (paper VI) all the most popular cosmological Nbody algorithms (PM, P^3M , adaptive P^3M , the tree-code and the adaptive multigrid code) are compared in respect to gravitational collisions that are caused by representing the continuous distribution of matter by discrete particles. For this a new measure of the two-body relaxation is used which is based on accumulated orbital deflection angles of particles. The analyis shows that in the P^3M type code the role of gravitational collisions is rather high, an unexpected fact that will force us to take the results of the simulations made using the P^3M with caution. The adaptive multigrid method is much better in this respect, but care is needed when finding the forces near subgrid boundaries; the force errors could also lead to enhanced orbital deflections, although to a much smaller extent that the gravitational collisions of discrete particles in the P^3M -method. This also shows that multigrid methods are certainly better to model the formation of structure (in dark matter) than other presently popular methods of simulation.

Chapter 1

Cluster Analysis of the Nonlinear Evolution of Large-Scale Structure in an Axion/Gravitino/Photino-Dominated Universe

The dynamically indicated but unseen "missing mass" in astrophysical systems has been an unresolved problem for half a century [1,2]. Nucleosynthesis arguments make nonbaryuonic particles an attractive hypothesis, with massive neutrinos a leading candidate.

Damping in neutrino-dominated universes [4,5,6] removes density perturbations smaller than $\lambda_c = 2\pi/k_c$; for m_{ν} 30 eV such a scale is characteristic of superclusters. Thus the primordial power spectrum is preserved up to a sharp cutoff. Gravitational collapse in such a universe is anisotropic and may lead to formation of galaxies from fragmentation of these structures [7]. We call this the adaiabatic (A) theory [7]. Simulations of the A theory with massive neutrinos indicate that galaxy/halo formation is possible and the structure compares reasonable well with observed large-scale structure of the universe [9-20]. A problem has been arisen in the analysis of structure in the A theory, however. The value of γ in the two-point correlation function $\xi(R) \propto R^{-\gamma}$ attains its observed value 1.8 only for short time after the collapse of structure, but galaxies must have formed at an early epoch [15-17]. Therefore one cannot simultaneously have the proper slope γ and have galaxies form long before the present, if this result is accepted. However, it should be mentioned that this result was obtained by ignoring dissipation, which could affect it. The observed γ is determined from galaxy counts, but the simulations to date include only "neutrinos."

Preceding this, there were numerical simulations [21, 22] of the hierarchical clustering theory (HC), in which galaxies form by coalescence of smaller subunits, and in turn cluster to form larger ones [23]. In this case it is assumed that the primordial power spectrum of density perturbations was undamped and so retains its primordial slope. HC simulations have been able to reproduce the $\gamma \sim 1.8$ [21] value but only at high amplitudes [22]. It seems that the proper large-scale structure is not produced [20, 24], in that statistical measures show too little "filamentary" character, as we will explain later.

Gravitinos [25-27] and photinos [28] are also attractive candidates for missing mass. Decoupling earlier, they have a lower present number density than relic neutrinos and may have larger masses and cluster in smaller systems. This is an attractive property if observations show that hidden mass exists in dwarf galaxies [29, 30] or in galactic disks [31]. Axions are bosons "created cold" which in spite of low mass may dominate galaxies and the universe through their high number density [32, 33].

It is usually assumed that primordial density perturbations followed a power law

$$|\delta_k|^2 \propto k^n, \tag{1.1}$$

where δ_k are the Fourier components of density. One can then write the density contrast on scale k_i as

$$(\delta\rho/\rho)_{k_i}^2 \propto \int_0^{k_i} k^2 |\delta_k|^2 dk, \qquad (1.2)$$

or

$$(\delta\rho/\rho)_{k_i} \propto k^{3/2+n/2}.\tag{1.3}$$

Undamped perturbations in a neutrino universe have almost uninterrupted growth, so that (in the linear regime) the slope of the power spectrum is preserved for $0 < k < k_c$. In an axion-, gravitino-, or photinodominated universe (AGP) there exists a time for which they are nonrelativistic but do not yet dominate. Perturbations entering the horizon during this period grow very little until they dominate. The resulting power spectrum is like the neutrino case for $0 < k < k_b$, but is "bent" to about n - 4for $k_b < k < k_c$. The scale k_b is determined by the horizon at the time when nonrelativistic species come to dominate, and for reasonable values of the present mass density and microwave temperature corresponds to supercluster scales, as does k_c for neutrinos. The free-stream damping scale k_c may be of galactic scales for gravitinos or photinos but is much smaller for axions or other cold particles. The shape of the power spectrum (except the value of k_c) is very general, and will arise for any sort of relic particle which is nonrelativistic before it begins to dominate the mass density of the universe. (The generic neutrino shape arises for "hot" particles, for which $k_b \sim k_c$.) For numerical results of calculations of these spectra, see the work of Bond, Szalay and Turner [26].

Thus on large scales AGP universes possess a similar structure which resembles neither that of the A nor the HC theory (unless $n \ge 3$, in which case it resembles HC) [33]. If n < 1 perturbations diverge on large scales without an *adhoc* cutoff. The n = 1 spectrum [34-36] is scale-free and emerges naturally from consideration of some inflationary universe schemes [37-41], and we adopt this spectrum for our simulation.

It is sometimes stated, on the basis of (1.3) that for n = 1 (bent to -3) all scales $k_b < k < k_c$ go nonlinear at once. However, (1.2) increases logarithmically. This increase is accentuated by the fact that the freezeout is not perfect, and power on galactic scales may grow by a small amount [26, 33]. This means that galactic scales collapse at a cosmic expansion factor six or more times smaller than that of the collapse of supercluster scales for our assumed spectrum.

The effective spectral index on small scales is then $n_e \sim n-4$. this is in accord with the conclusion that $n_e < -1$ which is based on cooling of gas to form galaxies [42]. For $n_e \sim -3$, energy per unit mass in bound systems is proportional to the size of the systems [43,44] which agrees with observation [45].

We have simulated the nonlinear evolution of structure in an AGP universe using the "bent" power spectrum described earlier as the initial condition for a cloud-in-cell (CIC) [46] gravitational clustering code. This code is an outgrowth of earlier work [10–13]. It uses one cloud per cell on a 32^3 mesh, but higher-resolution work is planned. In any case it will not be possible to resolve both k_b and k_c in such a code; we optimize the strength of the method, and study AGP universes in large-scale structure. We compare to an A model using the same code, and to the observations. The power spectrum of the two models was initially the same up to a value (k_b in AGP = k_c in A) beyond which there was a sharp cutoff in A and a bend to n = -3 in AGP.

We wish to emphasize that our conclusions depend on two approximations: (1.1) The gradual bend from n = 1 to n = -3 is approximated by sudden bend. (1.2) CIC codes accurately model large-scale collective modes but do not follow small-scale dynamics. It should be mentioned in regard to (1.2) that direct N-body methods follow small scales at the cost of introducing spurious noise on these time scales. This CIC code follows the dynamics accurately to $k \sim 2k_b$, and with decreasing accuracy to $k \sim 4k_b$. Thus we confine our attention to large-scale structures only. Also, smaller-scale structure will be affected by gas-dynamical processes.

In AGP the covariance function [47] $\xi(R)$ steepens as in the A model, but the AGP model attains the observed value ~ 1.8 just about at the time of structure formation on scale k_b . The amplitude of ξ at this time suggests that $\lambda_b \sim 40$ Mpc (pc \equiv parsec). If the covariance function is correctly calculated in the absence of hydrodynamics, this says that largescale structure is now pancaking, but galaxy formation may have proceeded at $Z \geq 5$ which removes a difficulty associated with the A model. Structures collapsing at this epoch could have radii ~ 100 kpc and densities ~ 10^{-25} g cm^{-3} , interestingly close to the characteristics [2] of galactic halos.

The density of an x-dominated universe, where x denotes a hypothetical particle, may be written as $\Omega h^2 = 7 \times 10^{-2} (m_x/1eV) g^{-1} g_x$, where Ω is the ratio of density to critical density, h is the Hubble constant in units of 100 km $s^{-1} M p c^{-1}$, m_x is our particle mass, g_* is the total effective number of degrees of freedom in all relativistic species at x decoupling, and g_x is the effective number of degrees of freedom in x [25, 26]. The scale λ_b is $(510 \text{ Mpc})(m_x/1eV)^{-1}g_*g^{-1}$ [26]. We therefore have the relation $\lambda_b \sim (36Mpc)/\Omega h^2$; our ~ 40 Mpc result from the simulation is compatible within the uncertainties to the observational bound $\Omega h^2 < 2$. This resolves a possible scaling problem [16, 48] which existed in neutrino (A) simulations, in that it seemed that Ωh^2 would exceed this bound if galaxy formation proceeded at $Z \geq 4$, as observations seem to require. The value 40 Mpc is characteristic of observed superclusters.

Visual inspection of particle position plots shows that the AGP model has a coherent structure on the scale k_b , in common with A models. Filamentary structures and voids are common in the AGP model, but there are some condensations in low-density regions. The AGP structure is more fragmented in appearance than the A structure. Galaxies may form in the voids but could possibly survive as dwarf galaxies and escape observation. Most matter collects in the coherent structure.

The function ξ cannot distinguish a nonlinear filamentary structure from an unclustered population [49], but the method of cluster analysis is able to do so [50]. In our approach two points are considered "neighbors" if their separation is less than neighborhood radius r_n . The principle "any neighbor of my neighbor is a neighbor of mine" is used to define connected structures.

The mass-weighted differential multiplicity function f(n) defined here

as the fraction of galaxies in systems of memebership n - dn to n. Previous studies showed that a simple hierarchical clustering model [51] strongly disagreed with observation in this respect. "A" simulations agreed rather well. It is not yet certain whether HC numerical simulations agree.

A characteristic size may be defined as the maximum distance between any two members of the same structure for given r_n . When a single structure spans the system, we say that percolation has taken place at neighborhood radius r_C [52]. We scale the radius to the radius of a sphere containing on average one particle.

There must be some unclustered primordial population. We exclude from consideration all particles not connected at neighborhood radius 0.89, the virial radius for two initial diagonal neighbors in a CIC code; this conservatively rejects (15-25)% of material as pregalactic.

The percolation parameter $B_C = (4\pi/3)r^3$ is found to be 1.15 in observed samples, with an error of a factor of 2 possible as a result of magnitude-limited samples and local density enhancement [50]. It is easily possible to fit this value and have $\gamma \sim 1.8$ in both A and AGP models. The simple hierarchical clustering model has $B_C \sim 5 - 11$, and a Poisson distribution has $B_C \sim 2.7$ [50]. For the A model we find a range 0.44 to 2.01, and for the AGP model 1.01 to 2.01.

We have studied the mass-weighted differential multiplicity function as it varies with time and r_n in both models. We find that the distribution of small, intermediate, and large systems is acceptable at the same time that the covariance function and percolation parameter are also.

It should be mentioned that while large-scale perturbations (above dipole) of the microwave background are of amplitude $\sim 2 \times 10^{-5}$ in a neutrino-dominated A model [53, 54], amplitude $\sim 3 \times 10^{-6}$ is expected in this AGP model [27], which is far below current sensitivity, and thus consistent with upper limits at present.

To sum up, it seems that the AGP universe shares many properties of the A universe which agree with observation. In addition, a possible problem of the A (neutrino) model is solved. The AGP universe with the scale-free primordial spectrum has intensive galaxy formation at $Z \ge 5$ (depending on details of the particle physics), comfortably early enough to account for galaxy/quasar evolution, as compared with the time that the covariance function attains slope $\gamma \sim 1.8$, and is compatible with constraints on Ωh^2 .

We stress that our conclusions depend on the power spectrum used, nit the specific particles. Nevertheless, we see here strong support for the structure formation process in an axion-, gravitino-, or photino-dominated universe. Galaxy formation proceeds from collapse of small-scale perturbations, as in the HC theory, but large-scale coherent structures forms as in A. The details of such a universe merit further study.

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Chapter 2

Theory of Lagrangian singularities and standard initial velocity fields

2.1 Introduction

Although the problem of the nature of dark matter is not solved yet, it is clear that it behaves non-dissipatively, interacting with itself and with other types of matter through gravitation. Estimates of the dark matter density show that it is much higher than that of the luminous matter, especially at scales of superclusters of galaxies and larger. Consequently one can say that the evolution of luminous matter at such large scales is determined by the self-gravitating collisionless motion of dark matter.

We are interested in the evolution of the spatial density distribution. Intuitively it is clear that it should be possible to find a geometrical classification of developed objects. For example, observational data and numerical models of the large-scale structure of the Universe show chains, surfaces and a small number of nearly spherical concentrations of matter. It is also clear that the formation of the structure elements should depend on the initial velocity field. On another hand, one can find an infinite number of different initial velocity fields that will produce qualitatively equivalent distributions of matter. This means that for classification of formed objects it is necessary to purge unimportant perturbations from the initial velocity field and to find standard fields that describe in some sense the generic situation. The latter requirement means that in case of small perturbations of the initial vector field the resulting matter distributions should be topologically equivalent.

It is possible to derive these standard vector fields using the theory of singularities of smooth mappings or, in case of mechanical systems, the theory of singularities of Lagrangian mappings.

These theories are local and do not include the physical scale of a grav-

itating system nor the time scale. Such flows of matter could exist locally during the formation of the large-scale structure of the Universe, because at this time there are few restrictions on the velocity field.

Much work has been done to numerically simulate the formation and evolution of the large-scale structure of the Universe. In these studies the main object of investigation has been the evolution of the power spectrum of density perturbations and of the correlation function of the matter distribution. Both of these statistics are insensitive to the geometry of the formed structure. The evolution of the geometry of the large-scale structure has remained unstudied so far.

To understand the processes that lead to the formation of structure in a generic matter distribution we shall abandon first the cosmological background and shall investigate the types of structure that develop from a general motion of particles.

Let us suppose that the initial velocity field is a smooth vector field. With this we restrict ourself to non-dissipative systems, where shock waves and stochastic motions (turbulence) do not occur. In this case the motion of particles can be described using a smooth function y = f(x,t), where y is the particle coordinate at the time moment t and x labels different particles. Initially the function f desribes an one-to-one mapping, but as time passes, particles start to catch up each other and density goes to infinity at the points in space, where the derivative of the function f with respect to the Lagrangian coordinate x is zero. The theory of Lagrangian singularities states that around such singular points x the function f can be transformed to a standard polynomial form using a smooth change of independent variables. Because the terminology and ideas of this theory are not common in astronomical literature we shall give in the following a short overview of the theory.

First we review the catastrophe theory that describes singularities of smooth functions from a generic point of view. Afterwards we define Lagrangian mappings, describe the types of singularities and bifurcations they can possess and at the end we find standard initial velocity fields using results of the theories mentioned above.

Investigation of the dynamical evolution of such standard fields could give us the classification of the possible types of dark matter distribution in superclusters of galaxies. If we include additionally gasodynamical effects, it should enable us to build both geometrical and dynamical models of observed superclusters of galaxies.

2.2 Singularities of smooth functions

Collisionless motion of particles can be described with smooth functions. Thus one can use general properties of smooth functions for description of different types of motion of matter.

For the classification of different types of motion we need a certain relation of equivalence or, speaking about smooth functions, it is necessary to define a relation of equivalence of these functions. We are interested in a local geometrical equivalence of graphs of smooth functions. For example, it is known that if a graph of a function has a saddle point, then in case of one-to-one change of coordinates this point remains a saddle point. The geometrical character of features of graphs of smooth functions is invariant under one-to-one transforms of coordinates; this gives us the definition of equivalence we are looking for.

Let us consider two smooth functions f(x) and g(x). These functions are equivalent if there exists a coordinate transform y(x) that

$$g(x) = f(y(x)) + \gamma.$$
(2.1)

We are interested in the local behaviour of functions, so from now on we drop the constant γ (it is possible to get rid of it by shifting the origin of coordinates). We study the behaviour of functions around the origin of coordinates and we suppose that f(0) = 0. We apply the following restriction on the coordinate transform y(x): y(x) should be smooth and it should have an inverse function. Transformations with such properties are called diffeomorphisms. These transformations itself have no singularities and so the change of coordinates does not add singularities to the original function.

The local behaviour of a smooth function is determined by its derivatives at a current point. Let us consider a function f of n variables. This defines a mapping $f: \mathbb{R}^n \to \mathbb{R}$ of n-dimensional space to 1-dimensional space of real numbers. Let us suppose that at the origin of coordinates $\nabla f \neq 0$, where

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \cdots, \frac{\partial f}{\partial x_n}\right). \tag{2.2}$$

The theorem of implicit function states that in this case there exists an inverse function for f. Consequently one can extend f up to a local diffeomorphism $g: \mathbb{R}^n \mapsto \mathbb{R}^n$ and

$$g(x) = (y_1 = f(x), y_2 = x_2, \cdots, y_n = x_n), \quad x, y \in \mathbb{R}^n.$$
 (2.3)

In this coordinate system the function f can be written as

$$f(y) = y_1.$$
 (2.4)

At every point where $\nabla f \neq 0$, the function f can be transformed to this standard form. Geometrically this means that at these points any function can be replaced by a linear function.

A smooth function has singularities at places where $\nabla f = 0$. Let us introduce some more definitions.

Consider a smooth function $f: \mathbb{R}^n \mapsto \mathbb{R}$. The point $u \in \mathbb{R}^n$ is a critical point if

$$\nabla f|_u = 0. \tag{2.5}$$

The value of a smooth function at a critical point f(u) is the critical value of this function. When n = 2 the tangent plane to the graph of a function f(x, y) at a critical point is parallel to the coordinate plane (x, y). For example, $f = x^2 + y^2$ has at the origin of the coordinate system a critical point called maximum, $f = -x^2 - y^2$ — a minimum, $f = x^2 - y^2$ — a saddle point.

A critical point is isolated if there are no other critical points around it. The critical points of functions listed above can serve as examples of isolated critical points. But there exist functions which have one or two lines of critical points. For example the function $f = x^2$, defined on the two-dimensional plane (x, y), has critical points lying on the y-axis, and for $f = x^2y^2$ both coordinate axes x, y are critical lines.

An important characteristic of a critical point is its degeneracy. We say that a function f has a non-degenerate critical point u if $\nabla f|_u = 0$ and the Hessian

$$Hf|_{u} = \left[\frac{\partial^{2} f}{\partial x_{i} \partial x_{j}}|_{u}\right]$$
(2.6)

is non-degenerate, that means that the determinant of the Hessian

$$det(Hf|_u) \neq 0. \tag{2.7}$$

It is possible to show that a non-degenerate critical point is isolated, but the opposite statement is not valid.

In the neighborhood of a nondegenerate critical point a smooth function can be transformed to a standard form by a smooth coordinate change. This follows from the following lemma.

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Morse Lemma: suppose that a smooth function $f : \mathbb{R}^n \to \mathbb{R}$ has a nondegenerate critical point at a point u. Then in the neighborhood U of point u it is possible to find a local coordinate system (y_1, \dots, y_k) , where $y_i(u) = 0$ for every i so that the function f can be expressed in the form

$$f = f(u) - y_1^2 - \dots - y_l^2 + y_{l+1}^2 + \dots + y_n^2$$
(2.8)

for all $u \in U$.

If we shift the origin of coordinates so that f(u) = 0, then it follows from this lemma that in the neighborhood of a non-degenerate critical point any function f can be expressed by a quadratic form.

Functions in the form $z_1^2 + z_2^2 + \cdots + z_{n-l}^2 - z_{n-l+1}^2 - \cdots - z_n^2$ are called Morse *l*-saddles. If l = n, the saddle is a maximum and if l = 0 — a minimum.

The Hessian of a Morse function is non-degenerate, as the number of independent variables z_i is equal to the rank of the quadratic form. At a non-Morse critical point the Hessian is degenerate. One can use as a quantitative measure of degeneracy the co-rank of the Hessian that is equal to the number of independent directions the Hessian is degenerate in. Consequently, at a degenerate critical point a function does not depend quadratically on all coordinates. The exact statement is given by the following lemma.

Splitting Lemma: let us have a smooth function $f : \mathbb{R}^n \mapsto \mathbb{R}$ and $\nabla f|_u = 0$. If the rank of this function at the point 0 equals r (and the co-rank is n-r), then f is equivalent around the 0-point to the function

$$f(x_{r+1}, \cdots, x_n) \pm x_1^2 \pm \cdots \pm x_r^2.$$
 (2.9)

This means that there exists a smooth coordinate transform that allows at a degenerate critical point to separate the degenerate part of a function that depends on n-r variables, and the non-degenerate (Morse) part that depends on r variables. The number r is the rank of the Hessian. When investigating the behaviour of a smooth function at a degenerate critical point we can ignore in the future the Morse part of the function and can concentrate our attention on functions with a smaller number of dependent variables, where the number of "bad" coordinates equals the co-rank of the Hessian of the original function at the degenerate critical point.

2.3 Families of smooth functions

Until now we have considered single functions. Let us turn our attention now to functions that depend, in addition to natural coordinates, also on parameters: $f: \mathbb{R}^n \times \mathbb{R}^l \mapsto \mathbb{R}$ (*l* is the dimension of the parameter space). For example, the function y = f(x, t) connects the initial coordinate of a moving particle with its final coordinate at the moment *t*. Here \mathbb{R}^n is the 3-dimensional physical space, but the time *t* plays the role of a parameter. Instead of a static picture we have a family of functions. At fixed parameter values the functions here are individual and all that was said in the previous chapter is applicable to them. The main difference is that the geometry of singularities can change qualitatively (metamorphosis of singularities) with the change of a parameter. The subject of the catastrophe theory is to describe such functional dependencies of families of functions on their parameters that the qualitative change of the local behaviour of individual functions proceeds in a structurally stable way. This means that close families evolve qualitatively similarly.

Let us start from the definition of the equivalence of families of functions (the classification of normal forms of families of functions is based on this notion). As in case of smooth functions we say that two families of functions, f and g, are equivalent in some neighborhood of zero, if there exist functions e, y, γ that

$$g(x,s) = f(y_s(X);e(s)) + \gamma(s),$$
 (2.10)

for every $(x,s) \in \mathbb{R}^n \times \mathbb{R}^l$ in this neighborhood. These functions should satisfy the following requirements:

- 1. $e: R^l \mapsto R^l$ is a diffeomorphism,
- 2. $y: R^n \times R^l \mapsto R^n$ is such a smooth mapping that for every $(x, s) \in R^n \times R^l$ in this neighborhood

$$y_n: R^n \mapsto R^n, \quad y_s(x) \equiv y(x,s)$$

is a diffeomorphism,

3. $\gamma: \mathbb{R}^l \mapsto \mathbb{R}$ is a smooth mapping.

From this definition we see that equivalent families of functions differ by families of diffeomorphisms of the coordinate space, by a diffeomorphism of the parameter space and by a shift function that is defined in the parameter space. Such transforms change local scales in \mathbb{R}^n and \mathbb{R}^l , but the qualitative character of singularities of a family is conserved.

The notion of the structural stability of a family of smooth functions emerges naturally now. If $f: \mathbb{R}^n \times \mathbb{R}^e \mapsto \mathbb{R}$ is equivalent to any family $f+p: \mathbb{R}^n \times \mathbb{R}^e \mapsto \mathbb{R}$, where $p: \mathbb{R}^n \times \mathbb{R}^e \mapsto \mathbb{R}$ is a small enough family (in a sense that the values of the functions around zero are close to zero), then f is structurally stable.

Structurally stable families of functions are in some sense typical (generic). In case of a small perturbation of such a family the geometrical evolution of the family with the changed parameters is qualitatively similar to that of the initial family. In order to describe equivalent families we introduce the notion of transversality. Consider a curve and a surface in a 3-dimensional space. If the curve intersects the surface, then this situation is stable against a small change of the curve. The point of intersection can move, but the fact of intersection by itself is conserved. The same situation happens when the curve does not intersect the surface anywhere. In case of a small displacement of the curve the property "the curve does not intersect the surface" is conserved. In such situations it is said that the curve and the surface are transversal. The relative position of a curve and a surface is unstable when the curve is tangential to the surface. Any small displacement of the curve either moves it off from the surface or the curve intersects the surface (a non-transversal situation). Transversality describes the geometrically generic situation. If one takes randomly a curve and a surface from the 3-dimensional space, then it is extremely probable that they are transversal. Non-transversal situations are very rare.

Other examples of transversality in the 3-dimensional space are two non-intersecting curves, two points and a curve that does not pass through a point. Examples of non-transversal situations are two curves tangent to each other, etc.

We see that transversality depends on the dimension of the space of objects (the manifold) and on the dimension of the space where these objects are defined. In a general case, if there exist two submanifolds X, Y in the space \mathbb{R}^n and dim X = s, dim Y = t, then X and Y are transversal if

- 1. $X \cap Y = \emptyset$ (non-intersecting),
- 2. dim $X \cap Y = max(0, s + t n)$ (intersecting),
- 3. X and Y are not tangent to each other.

Let us apply now the notion of transversality to families of functions.

Consider a functional space where the coordinates are the coefficients of the Taylor expansion. Every function is described as a point in this infinite-dimensional space. The degeneracy of a critical point connects the coefficients of the Taylor expansion by a certain relation that defines a hyper-surface in the functional space. In the simplest case the dimension of this surface of "special cases" is one less than the dimension of the whole space (the co-dimension of a surface is one in a 3-dimensional space). The really important number here is the co-dimension of the manifold of the special cases, so for simplicity we consider only a 3-dimensional space. With such a reduction of dimensionality the condition of transversality $\dim X \cap Y = \max(0, s + t - n)$ holds, because it includes the co-dimension codimY = n - t that is conserved.

It is clear that in general a function does not have degenerate critical points. A point on a surface in a 3-dimensional space is not transversal. This means that generic functions have only Morse critical points (in our 3-dimensional functional space these functions that are not lying on the surface of degenerate cases are described by points).

The coefficients of the Taylor expansion of families of functions depend on the parameters of a family. Consequently with the change of parameters a point draws a curve in the functional space, a surface draws a hypersurface and etc., depending on the number of parameters.

In general this hyper-surface of a family can intersect the surface of special cases. So families of functions could include functions with degenerate singular points in a generic case. The stability of the formation of such points in families of functions is determined by transversality of the surface of the family to the surface of degeneracy.

So we can define the structural stability of families of functions as transversality of the surface of the family to the manifold of special cases in the functional space.

Transversality by itself is a stable property. Intuitively it is clear that transversal intersections are locally qualitatively similar (they depend only on the dimension of the intersecting hyper-surface at the current point). Thus it should be possible to transform the form of intersection to a standard form at every point of intersection with a local coordinate change. This means that the canonical form of a family of functions should consist of two parts: a canonical form of functions which have a degenerate critical point, and a canonical form of functions which depend on parameters and describe the transversal path through the hyper-surface of degenerate functions.

Let us define now the canonical form of a family of functions which have a degenerate critical point at the origin of coordinates. According to the splitting theorem of families of functions we can transform a family $f: \mathbb{R}^n \times \mathbb{R}^l \mapsto \mathbb{R}$ in the vicinity of a degenerate critical point by a local diffeomorphism to the form

$$\tilde{f}(x_1, \cdots, x_m) \pm x_{m+1}^2 \pm \cdots \pm x_n^2,$$
 (2.11)

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where m is the co-rank of the Hessian

$$H\hat{f}|_{0} = \left[\frac{\partial^{2}\hat{f}}{\partial x_{i}\partial x_{j}}|_{0}\right].$$
 (2.12)

Let us consider in the following the family \hat{f} that depends on the "bad" coordinates x_1, \dots, x_m and the parameters $c \in \mathbb{R}^l$. Suppose that a degenerate critical point appears at c = 0. With this we separate from the family a function that has a degenerate critical point at the origin of coordinates $x = 0, x = (x_1, \dots, x_m)$. We can write the function $f : \mathbb{R}^n \to \mathbb{R}$ formally in the form

$$f = j^k f + Tayl, (2.13)$$

where $j^k f$ is the k-jet of the function (a section of the Taylor expansion from the first term until the kth, the latter included) and Tayl is the remaining tail of the expansion. For many functions there exists a value k at which the inclusion of higher order terms does not change the qualitative behaviour of the function. It is said that the function f is k-determined, if its k-jet is equivalent to any function of the form f + g, where g is a polynomial of rank k + 1.

Local equivalence allows us to use the infinitesimal coordinate transformation

$$y^{t}(x) = x + tq(x), \quad t \ll 1,$$
 (2.14)

where q(x) is a polynomial with a minimal exponent ≥ 2 . Under this coordinate change the point $j^{k+1}f$ draws a trajectory (the orbit of the (k + 1)-jet) in the functional space. Differentiation gives us the tangent velocity vector

$$v^{k+1} = j^{k+1} \left(q(x) \frac{\partial f}{\partial x} \right).$$
(2.15)

In a multi-dimensional case for the transform

$$(y_1, \cdots, y_n) = (x_1 + tq_1(x), \cdots, x_n + tq_n(x)), \quad x = (x_1, \cdots, x_n)$$

(2.16)

we get the set of tangent vectors

$$v_i^{k+1} = j^{k+1} \left(q_i \frac{\partial f}{\partial x_i} \right) = \left[Q_i(x) \frac{\partial f}{\partial x_i} \right]^{k+1}, \qquad (2.17)$$

where $Q_i(x)$ is a polynomial with a minimal exponent ≥ 2 . These vectors form a tangent space to the orbit of $j^{k+1}f$ under the group of infinitesimal coordinate transformations. The notation $[A]^l$ means the truncation of a polynomial up to the *l*-order term.

If this tangent space coincides with the tangent space of the sub-mani-fold of all (k + 1)-jets whose k-jet equals $j^k f$, then these manifolds are identical. In this case we can, using a local coordinate transform, obtain any jet $j^{k+1}f$, among them also these where the coefficients before the k + 1-order term are equal to zero.

The condition of the coincidence of the tangent space with the space of terms with the exponent k + 1 is fulfilled if the dimensions of these spaces are equal. Thus the function f is k-determined, if any polynomial of the order k + 1 can be expressed in the form

$$\sum_{i=1}^{n} \left[Q_i \frac{\partial f}{\partial x_i} \right]^{k+1}.$$
(2.18)

This means that by a coordinate change it is possible to remove all terms with the exponent k+1 from the Taylor expansion of the function f. In the same way it is possible to throw away all terms of its Taylor expansion with exponents higher than k. In other words, the behaviour of a k-determined function is defined by its k-jet.

Let us study now the remaining part of the jet. Vectors (3.8) define the tangent space to the (k+1)-jet of the function. Let us denote this tangent space by $\delta_{k+1}(f)$. It forms the sub-space of the general space of (k+1)-jets J_n^{k+1} , where the basis vectors are all kinds of terms like $x_{i_1}^{k_1} \cdot \ldots \cdot x_{i_l}^{k_1}$, where $l \leq n, k_1 + \cdots + k_n \leq k+1$ and $i_m \leq n$.

If the dimensions $\delta_k(f)$ and J_n^k are not equal, then this means that some directions in the k-jet of the current function are absent. We define the codimension of a function as $codimf = (\dim J_n^k - \dim \delta_k(f))$ (the number of absent directions in the functional space).

The co-dimension of a function is naturally connected to the co-rank of the Hessian at a degenerate critical point. Using the splitting theorem it is possible to separate "bad" and "good" variables:

$$f(y) = \hat{f}(y_1, \cdots, y_m) \pm y_{m+1}^2 \pm \cdots \pm y_n^2, \qquad (2.19)$$

where *m* is the co-rank of the Hessian and $j^k f$ is a polynomial that does not include terms with the exponent less than 3 (the quadratic terms will be in the Morse part of the function). The tangent space $(\partial f/\partial x_{m+1}, \cdots, \partial f/\partial x_n)$ to the Morse part of the function includes linear terms, so all directions in J_n^k (k = 2 in current case) can be expressed in the form of linear combinations $\sum_i g(y)y_i, m+1 \le i \le n$, where g(y) is a polynomial. There are no quadratic terms in the degenerate part of the function \hat{f}

There are no quadratic terms in the degenerate part of the function \hat{f} and the tangent space to $j^3 \hat{f}$ does not include directions that correspond to the linear and quadratic directions in J_n^3 . The number of the last is m + m(m+1)/2. Consequently

$$codim\hat{f} = m + \frac{m(m+1)}{2} - m = \frac{m(m+1)}{2}.$$
 (2.20)

If some directions in $\delta_3(f)$ are linearly dependent, then $\dim \delta_3(\hat{f}) \leq m$ and we have

$$codim\hat{f} \ge \frac{m(m+1)}{2}.$$
 (2.21)

Thus, if a function is k-determined, then it is possible to truncate its Taylor expansion to the k-jet $j^k f$. It is possible to split a function to its degenerate and non-degenerate parts at a degenerate critical point and in this case the second derivative of the degenerate part of the function is equal to zero (the Hessian is degenerate). Accordingly, the k-jet of the non-Morse part of the function does not include quadratic terms. Such a section of the k-jet is called the germ of the function. The equivalence of germs is defined similarly to the equivalence of functions. It is possible to transform germs to a canonical form and to classify them by the co-rank (the number of "bad" coordinates) and by the co-dimension of the germ at a degenerate critical point.

The transformation of the germ of a function to a canonical form proceeds as follows. At the current co-dimension s there are no first s terms in the jet, starting from quadratic. One could try to transform the remaining part of the germ to a normal form, using a linear change of coordinates

$$y = Ax, \qquad (2.22)$$

where $A = (a_{ij})$ is a matrix with the dimension m^2 , where *m* is the corank of the Hessian. Choosing m^2 values of coefficients one can reduce to a normal form m^2 terms of a germ. But with the increasing co-rank *m* and the increasing number of terms to be killed in a jet it can happen that it is impossible to kill $m^2 + s$ terms together with the reduction of the remaining part of the row to a normal form (equal to one of the coefficients of the monomials of the expansion). These remaining free parameters are called moduli. In this case we do not have one concrete germ of a function, but a whole family of germs. Germs without moduli are called simple germs, and germs with moduli are complicated germs. For example in case of m = 2 and s = 7 we can throw away all quadratic terms $(x^2, xy, y^2, 3 \text{ in total})$ and all cubics $(x^3, x^2y, xy^2, y^3, 4 \text{ in total})$, but with $m^2 = 4$ coefficients of a linear transform it is impossible to reduce to the normal form the terms with the exponent 4 (there are 5 of them). Another example: m = 3, s < 6. Here the number of the cubic terms is larger than $m^2 = 9$.

So, it is possible to find a number of canonical forms of germs of functions $f: \mathbb{R}^n \mapsto \mathbb{R}$ at a degenerate critical point. Such points can exist in general only in families of functions. This means that it is necessary to add to a normal form of a function also its canonical dependence on parameters.

We extend the germ of f(x) up to a family F(x, c), where

$$F(x,0) = f(x),$$
 (2.23)

in the following way:

$$F(x,c) = f(x) + c_1 v_1 + \dots + c_r v_r, \qquad (2.24)$$

where r is the number of parameters. To get the family F(x, c) as a family of a generic situation, it is necessary that the hyperspace of the family, defined by the vectors v_i , should be transversal to the sub-space of "bad" directions of $\delta_k(f)$. The minimal number of parameters r is defined by the condition r = codimf. Such a family (deformations of a germ) is called an universal deformation. Any other family that has a degenerate critical point, the type of which is defined by the germ of f(x), can be obtained from the universal deformation.

From the condition of transversality it follows that the minimal basis for the universal deformation can be built from the co-basis of $\delta_k(f)$ in J_n^k , so for v_i we can choose directions in $(J_k^n - \delta_k(f))$.

We give as an example the determination of the universal deformation for the function

$$f(x,y) = x^{3}y + y^{3} + O(4).$$
(2.25)

As a starting point, we show that this function is 3-determined. Let us determine the tangent plane to the orbit of j^3f . It consists from linear combinations of polynomials of the form

$$\left[x_i^l \frac{\partial f}{\partial x_i}\right]^4. \tag{2.26}$$

We find

$$\frac{\partial f}{\partial x} = 2xy + O(3), \quad \frac{\partial f}{\partial y} = x^2 + 3y^2 + O(3). \tag{2.27}$$

Let us consider only combinations giving polynomials with the exponent of four:

$$\begin{bmatrix} x^2 \frac{\partial f}{\partial x} \end{bmatrix}^4 = 2x^3 y, \qquad \begin{bmatrix} x^2 \frac{\partial f}{\partial y} \end{bmatrix}^4 = x^4 + 3x^2 y^2,$$
$$\begin{bmatrix} xy \frac{\partial f}{\partial x} \end{bmatrix}^4 = 2x^2 y^2, \qquad \begin{bmatrix} xy \frac{\partial f}{\partial y} \end{bmatrix}^4 = x^3 y + 3x y^3,$$
$$\begin{bmatrix} y^2 \frac{\partial f}{\partial x} \end{bmatrix}^4 = 2x y^3, \qquad \begin{bmatrix} y^2 \frac{\partial f}{\partial y} \end{bmatrix}^4 = x^2 y^2 + 3y^4.$$

We see that the tangent space $\delta_4(f)$ has all terms with the fourth exponent $(x^3y, x^2y^2, xy^3, x^4, y^4)$. Consequently, this function is 3-determined. This means that there exists a coordinate transform that brings the initial function to the form $x^2y + y^3$.

Consider now the tangent space $\delta_3(f)$ to the orbit of the 3-jet of the function. It consists of all linear combinations of the form

$$\left[x_i^l \frac{\partial f}{\partial x_i}\right]^3. \tag{2.29}$$

We get

1

$$J_{1} = 2xy, \quad J_{2} = x^{2} + 3y^{2}, \quad J_{3} = \frac{1}{2}x(2xy) = x^{2}y,$$

$$J_{4} = \frac{1}{2}y(2xy) = xy^{2}, \quad J_{5} = x(x^{2} + 3y^{2}) - \frac{3}{2}y(2xy) = x^{3},$$

$$J_{6} = \frac{1}{3}y(x^{2} + 3y^{2}) - \frac{1}{6}x(2xy) = y^{3}.$$
(2.30)

Consequently, $\delta_3(f)$ has all basis monomials with the exponent three (x^3, x^2y, xy^2, y^3) , but one direction in the space of quadratic terms is absent $(xy, x^2 + 3y^2)$ gives two directions, but the full basis has 3 terms – x^2, xy, y^2).

The co-basis can now be chosen from the terms

$$v_1 = x, \quad v_2 = y \quad \text{and} \quad v_3 = x^2.$$
 (2.31)

The linear combinations of v_3 , J_1 , J_2 and J_3 give the terms of the quadratic basis

$$x^2 = v_3, \quad xy = \frac{1}{2}J_1, \quad y^2 = \frac{1}{3}(J_2 - v_3).$$
 (2.32)

At last we can write the universal deformation

$$f(x,y) = x^2y + y^3 + t_3x^2 + t_2y + t_1x.$$
(2.33)

All germs of small co-dimensions have been classified in a similar way. This result is known as a Thom's classification theorem.

A typical r-parameter function family $f : \mathbb{R}^n \times \mathbb{R}^r \mapsto \mathbb{R}$, where n and r < 5, is structurally stable and its germ around any point is equivalent to one of the following normal forms:

- 1. non-critical: x_1 ,
- 2. non-degenerate critical (or Morse): $x_1^2 + \cdots + x_l^2 x_{l+1}^2 \cdots x_n^2$,
- 3. fold (A_2) : $x_1^3 + t_1x_1 + (M)$,
- 4. cusp (A₃): $x_1^4 + t_2 x_1^2 + t_1 x_1 + (M)$,
- 5. swallowtail (A₄): $x_1^5 + t_3 x_1^3 + t_2 x_1^2 + t_1 x_1 + (M)$,
- 6. butterfly (A₅): $x_1^6 + t_4 x_1^4 + t_3 x_1^3 + t_2 x_1^2 + t_1 x_1 + (M)$,
- 7. elliptic umbilic (D_4^-) : $x_1^2x_2 x_2^3 + t_3x_1^2 + t_2x_2 + t_1x_1 + (M)$,
- 8. hyperbolic umbilic (D_4^+) : $x_1^2x_2 + x_2^3 + t_3x_1^2 + t_2x_2 + t_1x_1 + (M)$,
- 9. umbilic (D_5^+) : $x_1^2x_2 + x_2^4 + t_4x_2^2 + t_3x_1^2 + t_2x_2 + t_1x_1 + (M)$,

where (M) is the Morse part of the function.

The list given above exhausts all deformations of simple germs with r < 5. Germs which include the third coordinate x_3 are complicated, depending on a modulus.

A more detailed representation of the theory is given in (Poston et al. 1978, Gilmour 1981, Lu 1980).

2.4 Theory of singularities of Lagrangian mappings

In order to apply the catastrophe theory in mechanics it is necessary to restrict the class of spaces considered and of functions that are allowed. The corresponding theory is called the theory of Lagrangian mappings. This theory describes mappings that are defined in spaces that are similar to the phase space of Hamiltonian mechanics. By itself the theory of Lagrangian mappings does not need to refer to classical mechanics, as it uses only the geometrical properties of the phase space. But to show the physical essence of the theory it is better to explain it using the known terms of mechanics.

In the phase space of classical mechanics there are two types of coordinates; a general coordinate $q = (q_1, \dots, q_n)$ that defines the so-called configuration space, and conjugate with it the general impulse $p = (p_1, \dots, p_n)$. The phase space of a mechanical system with *n*-degrees of freedom itself looks like a \mathbb{R}^{2n} . The motion of a mechanical system in the configuration space is determined by the function of action

$$S(q,t) = \int_{t_0}^t L(q,\dot{q},t) dt,$$
 (2.34)

where L is the Lagrange function for a mechanical system. The trajectory q(t) of a material point is defined as a curve between the points (q_0, t_0) and (q, t) in the extended configuration space (q, t) that gives the minimum of the function of action along this curve. This principle of least action is expressed by the condition

$$\delta \Phi[\gamma] = \delta \int_{\gamma} L(q, \dot{q}, t) dt = 0, \qquad (2.35)$$

where $\delta \Phi$ is the variation of the functional $\Phi[\gamma]$ along the curve γ that connects the points (q_0, t_0) and (q, t). Lifting these curves to the extended phase space (p, q, t) one can get the principle of least action in the phase space. For this it is necessary to use the relation between the Lagrangian, defined in the configuration space, and the Hamiltonian of the same mechanical system, defined in the phase space:

$$H(p,q,t) = p\dot{q} - L(q,\dot{q},t), \qquad (2.36)$$

where the generalised momentum p and the velocity \dot{q} are related by the definition

$$p_i = \frac{\partial L}{\partial \dot{q}_i}, \quad 1 \ge i \ge n.$$
(2.37)

Consider now a functional of the form

$$\Phi[\gamma] = \int_{\gamma} (p\dot{q} - H)dt, \qquad (2.38)$$

where γ is the curve connecting the points (p_0, q_0, t_0) and (p_1, q_1, t_1) . We find the extremal curve γ relative to variations of γ , when the endpoints of
it are fixed at *n*-dimensional sub-spaces $(q = q_0, t = t_0)$ and $(q = q_1, t = t_1)$, in the (2n + 1)-dimensional extended phase space (p, q, t)

$$\delta \int_{\gamma} \left(\dot{q} \delta p + p \delta \dot{q} - \frac{\partial H}{\partial p} \delta p - \frac{\partial H}{\partial q} \delta q \right) dt = = p \delta q |_0^1 + \int_{\gamma} \left[\left(\dot{q} - \frac{\partial H}{\partial p} \right) \delta p - \left(\dot{p} + \frac{\partial H}{\partial q} \right) \delta q \right] dt = 0. \quad (2.39)$$

The first term in the sum is zero, because the endpoints of the curve are fixed in q. From the second term we find that the integral curves of the canonical Hamilton equations

$$\dot{p} = -\frac{\partial H}{\partial q}, \quad \dot{q} = -\frac{\partial H}{\partial p}$$
 (2.40)

are the extremals of the integral (4.5) in the class of curves γ , the endpoints of which are fixed on the sub-spaces $(q = q_0, t = t_0)$ and $(q = q_1, t = t_1)$. This means that the function of action can be expressed by

$$S(q,t) = \int_{t_0}^t (p\dot{q} - H)dt = \int_{q_0}^q pdq - \int_{t_0}^t Hdt.$$
 (2.41)

The function of action (4.8) determines the phase trajectories of a mechanical system with the hamiltonian H.

To investigate the pencil of such trajectories it is convenient to define in the phase space (p,q) some surface, like the graph of the function

$$p_i = f_i(q), \quad 1 \ge i \ge n, \tag{2.42}$$

that defines a *n*-dimensional surface in the 2*n*-dimensional phase space. The points of the surface, moving along a phase trajectory, form after time t a new smooth surface with the same dimension. Unifying these *n*-dimensional surfaces along time, we get a (n+1)-dimensional surface that consists of all phase trajectories starting from the initial *n*-dimensional surface. In other words, this (n+1)-dimensional surface is formed by the extremals of action S(q,t).

Along the extremals the function of action is an one-valued function of the endpoint of the extremal, so the differential of the action

$$dS = pdq - Hdt \tag{2.43}$$

is total. At a fixed time $t = t_0$, the section of the (n + 1)-dimensional surface of a pencil of trajectories gives a *n*-dimensional surface where the

differential of the truncated action $S_0(q) = S(q, t = t_0)$ is total: $dS_0 = pdq$ (on this surface dt = 0).

In general, a *n*-dimensional surface in a 2*n*-dimensional phase space (p,q) is called Lagrangian, if for all curves γ on this surface, the truncated action

$$S = \int_{\gamma} p dq \tag{2.44}$$

is a locally one-valued function, depending only on the endpoint of the path γ . Or equivalently, the graph of the function $p_i = f_i(q)$ is a Lagrangian surface, if

$$p_i = f_i(q) = \frac{\partial S}{\partial q_i}.$$
(2.45)

Using the analogy between mechanics and geometrical optics, one can say that a Lagrangian surface is similar to a wave front that is perpendicular to a system of light rays, and the gradient of the optical path-length gives the direction of motion p of the wave front.

For the following it is necessary to give generalisations of given definitions. We have shown that the Lagrangian surface can be defined by the gradient of the action function. In any space \mathbb{R}^m with coordinates y_1, \dots, y_m the gradient of a function has the form

$$(\nabla f)_i = \sum_j g_{ij} \frac{\partial f}{\partial y_j}, \qquad (2.46)$$

where g_{ij} is a non-degenerate matrix of metrics. The gradient of a function defines at every point of space a vector that can be identified with the velocity vector of the point

$$\dot{y}_i = (\nabla f)_i. \tag{2.47}$$

Dynamical systems of this type are called gradient systems. A special case of them is the Hamiltonian system

$$\dot{y}_i = (\nabla H)_i \tag{2.48}$$

or in the canonical coordinates p, q:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}.$$
 (2.49)

From this one can see that in the basis p_j, q_i the matrix of metrics has the form

$$g_{q_i p_j} = \begin{pmatrix} 0 & E \\ -E & 0 \end{pmatrix}, \quad E = \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix}, \quad (2.50)$$

so it is a skew-symmetric matrix.

Let us define now the n-dimensional Lagrangian surface by n equations

$$y_i = (\nabla F)_i \tag{2.51}$$

or

$$y_i = \sum_j g_{ij} \frac{\partial F}{\partial y_j}, \quad 1 \ge i, j \ge n.$$
(2.52)

Let us assume that the function F is defined in the phase space as $F = F(p_I, q_J)$, where $p_i = (p_1, \dots, p_l)$ and $q_J = (q_{l+1}, \dots, q_n)$. The set $(1, \dots, n)$ can be split into two disjoint parts in 2^n ways. So our generalised Lagrangian surface can be defined by one of the 2^n formulas of the form (Arnold 1972)

$$q_i = \frac{\partial F}{\partial p_i}, \quad 1 \ge i \ge l, \quad p_j = -\frac{\partial F}{\partial q_i}, \quad l+1 \ge j \ge n.$$

$$(2.53)$$

After such a generalisation the function F cannot be longer identified with a function of action. Anyway, the surface, defined in this way, can be considered as the instantaneous state of the pencil of trajectories of a gradient system.

Under the influence of the Hamiltonian phase flow the Lagrangian surface deforms, but remains Lagrangian. This is caused by the fact that the Lagrangian surface has a zero area of projection to the coordinate planes (p_i, q_i) ; the Lagrangian surface is defined by a locally one-valued function, but the area of a curve is zero. The Hamiltonian phase flow conserves the sum of areas of projections to the planes of conjugate coordinates (p_i, q_i) , $1 \ge i \ge n$. So the zero area remains zero, and the Lagrangian surface remains Lagrangian.

The simplest examples of Lagrangian surfaces are the planes $q = q_0$ (the momentum is undefined) and $p = p_0$ (the coordinates are undefined).

The Lagrangian surface is the central notion of the theory of Lagrangian mappings. From the definition of the first follows the definition of the second.

A Lagrangian mapping is the projection of the Lagrangian surface onto the configuration plane:

$$P(p,q) = q, \tag{2.54}$$

where p, q are the coordinates of a point in the phase space that satisfy the equation of the Lagrangian surface. Thus the Lagrangian mapping can be given by the first equation in (2.53) that defines the Lagrangian surface.

The projection gives the instantaneous state of the system in the configuration (ordinary) space. Choosing points on the Lagrangian surface, we shall get after projection the distribution of points in the configuration space. Under the influence of the Hamiltonian phase flow the Lagrangian surface deforms. It can happen that at some point of the surface the derivative $\partial q_i / \partial p_j = 0$. This means that the projection ceases to be locally onevalued and in the configuration space there forms a visual contour - the caustic. If one considers a particle system moving under self-gravity (e.g. the Hamiltonian depends on time), with an initial distribution of momentum and coordinates defined on the Lagrangian surface, then at the points of a caustic in the configuration space the density will be infinite in the approximation of a continuous medium. It is clear that at corresponding points of the Lagrangian surface the Hamiltonian (more precisely the potential energy) will be undefined together with the direction of the phase flow at these points. But until the appearance of the caustic, the whole motion of the system can be described by the deformation of the Lagrangian surface.

Consider now how one could obtain the normal form of the "generating function". If the co-rank of the Hessian

$$HF = \left[\frac{\partial^2 F}{\partial p_i \partial p_j}\right] \tag{2.55}$$

equals m, then in the equation (2.53) of the Lagrangian surface one can take l = m. The Lagrangian mapping can be considered as depending on the parameters of the projection of the surface with a small number of dimensions onto a plane. This is similar to the selection of the dependent "bad" coordinates of a function using the splitting theorem. Let us move the origin of coordinates by a shift in the q_J -plane into the point where the Lagrangian mapping has a singularity. Suppose that in $F(p_I, q_J)$ the p_I are natural coordinates, but q_J play the role of parameters. So, we have the family of functions and

$$F(0,0) = 0, \frac{\partial F}{\partial p_i|_{(0,0)}} = 0, \quad 1 \ge i \ge m.$$
(2.56)

From the point of Lagrangian mappings the last condition is not yet the condition for a critical point of a mapping. It simply means that at the origin of coordinates $q_J = 0$. Recall that Lagrangian singularities occur at the points where

$$\frac{\partial q_i}{\partial p_j} = \frac{\partial^2 F}{\partial p_i \partial p_j} = 0, \quad 1 \ge i, j \ge m.$$
(2.57)

It means that the second derivative of F equals zero and consequently the normal form of the function F can be expressed by polynomials that have exponents that are higher by one compared to the corresponding normal forms of functions of the catastrophe theory.

This analogy between the catastrophe theory and the theory of La-grangian mappings is external. The intrinsic difference between the theories follows from the difference of mappings and from the fact that they are defined in spaces with different properties. So it is natural that these theories differ by the definition of equivalence of mappings. In the catastrophe theory equivalent families of functions are produced using the diffeomorphism of the space of natural coordinates and of the space of parameters. In the theory of Lagrangian mappings only such diffeomorphisms of the phase space are allowed when the Lagrangian surfaces remain Lagrangian. This transform can be realised using the Hamiltonian phase flow, that conserves the zero volume of the Lagrangian surface. Consequently, the allowed diffeomorphisms should be canonical. In case of the Lagrangian equivalence, e.g. in case of a canonical transform of the phase space, a diffeomorphism occurs on the Lagrangian surface. The configuration space is connected to the Lagrangian surface by a projection (Lagrangian mapping), so a diffeomorphism on the Lagrangian surface induces a diffeomorphism in the configuration space. Consequently, from the Lagrangian equivalence there follows the equivalence of caustics (the set of the critical values of the Lagrangian mapping) in the sense of the ordinary catastrophe theory.

In order to determine the normal forms of structurally stable Lagrangian mappings the same methods are used as in the catastrophe theory, so the individual types of singularities coincide with similar types from the list of the previous section. We give now the classification of the normal forms of Lagrangian mappings.

Any *n*-dimensional Lagrangian surface can be transformed, using any small deformation in the class of Lagrangian surfaces, into such that the projection onto the configuration space will be at any point Lagrangian equivalent to a Lagrangian mapping of the form (Arnold 1980):

1. in case of n = 1

$$A_1: F = p_1^2, \quad A_2: F = \pm p_1^3,$$
 (2.58)

2. in case of n = 2

$$A_3: F = \pm p_1^4 + q_2 p_1^2$$
, and previous; (2.59)

3. in case of n = 3

$$A_4: F = \pm p_1^5 + q_1^3 + q_2 p_1^2,$$

$$D_4: F = \pm p_1^2 \pm p_2^3 + q_3 p_2^2, \text{ and previous;}$$
(2.60)

4. in case of n = 4

$$A5: F = \pm p_1^6 + q_4 p_1^4 + q_3 p_1^3 + q_2 p_1^2,$$

$$D5: F = \pm p_1^2 p_2 \pm p_1^4 + q_4 p_2^3 + q_3 p_2^2 \text{ and previous.}$$
(2.61)

In this list the Morse part of the function $F(p_I, q_J)$ that depends on the coordinates q_J is left out everywhere, as it is unimportant when studying typical singularities.

To summarize the theory of Lagrangian singularities we can say that under the influence of the Hamiltonian phase flow, the Lagrangian surface deforms, and a typical Lagrangian mapping has singularities from the list above. This means that when studying motion of particles, the singularities of the particle distribution, taken from the normal forms of caustics above, are structurally stable.

2.5 Metamorphoses of caustics

In the previous section we described the normal forms of Lagrangian mappings around simple critical points in spaces of small dimension. To study the evolution of singularities it is necessary to introduce the parameter of time, e.g. to consider the one-parameter family of Lagrangian mappings.

Let us consider the medium of non-interacting particles. The Lag-rangian surface can be expressed in the form $p = \partial S / \partial q$, that corresponds to a gradient distribution of momentum. The phase flow is obtained from the Hamilton equations

$$\dot{p} = 0, \quad \dot{q} = 0,$$
 (2.62)

where the first equation says that the flow is force-free.

The projection of the phase flow g(p, q, t) = q + tp onto the configuration space gives the equations of motion in it:

$$q(t) = q_0 + t \frac{\partial S}{\partial q}, \quad q_0 = q(t = t_0), \tag{2.63}$$

where S = S(q). The mapping $x \mapsto \partial f/\partial x$ is called a gradient mapping, a special case of a Lagrangian mapping. Any Lagrangian mapping is equivalent to a gradient mapping. We see that in the configuration space we have the one-parameter family of Lagrangian mappings.

We introduce now another, equivalent presentation of the above picture. Let us mark the coordinate q_0 , which is called Lagrangian in the fluid dynamics, by x, but the Eulerian coordinate q(t) by y.

The points from the x-space parametrize the individual particles of the matter, but the points from the y-space correspond to the location in space where the points are at the time moment t. Unification of spaces x and ygives us the space (x, y), similar to the phase space, where at every time moment the Lagrangian surface is defined by the mapping (2.63). Projection to the Eulerian space gives the distribution of matter at the time moment t. It is clear that the extended mapping $(x, t) \mapsto (y, t)$ gives us the whole picture of evolution of the distribution of matter. It can be shown that the large mapping $(x,t) \mapsto (y,t)$ is an one-parameter family of Lagrangian mappings (Arnold 1983). At a fixed time moment the Lagrangian mapping has a instantaneous caustic in the *n*-dimensional Eulerian space. When the time passes a certain critical value, the geometry of the caustic can change abruptly. To describe general metamorphoses of caustics in a *n*-dimensional space it is necessary to study general singularities of caustics in spaces with dimension higher by one, because the large mapping can be considered as a Lagrangian mapping onto a (n+1)-dimensional space. The set of all critical values of the large mapping consists of all instantaneous caustics, corresponding to different time moments.

During the reduction to a normal form of caustics in the Eulerian spacetime, all coordinates are equal. But in the extended Eulerian space the time coordinate is different from others in that it has only one direction. Consequently the instantaneous Eulerian spaces (isochrones) should be defined in the form of a function $t = f(y, \lambda)$ that does not have critical points. The

Туре	F	k	t
A_3	$x^4 + \lambda_1 x^2$	1	$\tau_1 \text{ or } \pm \lambda_1 \pm \tau_1^2$
A_4	$x^5 + \lambda_1 x^3 + \lambda_2 x^2$	1	$\pm\lambda_1$
D_4^{\pm}	$3x_1^2x_2 \pm x_2^3 + 3\lambda_1(x_1^2 \mp x_2^2)$	2	$\pm\lambda_1+y_1+ay_2$

Table 2.1: Metamorphoses of Lagrangian singularities, n = 2

* Here the components of λ are denoted as λ_i and τ_j .

Table 2.2: Metamorphoses of Lagrangian singularities, n = 3

Туре	F	k	t
A_3	$x^4 + \lambda_1 x^2$	1	$\tau_1 \text{ or } \pm \lambda_1 \pm \tau_1^2 \pm \tau_2^2$
A_4	$x^5 + \lambda_1 x^3 + \lambda_2 x^2$	1	$ au_1$ or $\pm\lambda_1\pm au_1^2$
A_5	$x^6+\lambda_1x^4+\lambda_2x^3+\lambda_3x^2$	1	$\pm\lambda_1$
D_4^{\pm}	$3x_1^2x_2 \pm x_2^3 + 3\lambda_1(x_1^2 \mp x_2^2)$	2	$ au_1$ or $\pm\lambda_1+y_1+ay_2\pm au_1^2$
D_5	$x_1^2 x_2 + x_2^4 + \lambda_1 x_2^3 + \lambda_2 x_2^2$	2	$\pm\lambda_1+y_1+ay_2$

reduction to a normal form of this function is carried out using a diffeomorphism that conserves the large caustic [7]. For singularities of type A, the reduction of the time function to a normal form is realized by a local diffeomorphism that conserves the caustic, and with addition of a constant. For singularities of type D, in addition to that, a transform t = t'(t) of the time-axis is used.

According to the paper (Arnold 1983) we list in Tables 2.1, 2.2 the normal forms of functions to what a general function $t(y, \lambda)$ without critical points can be reduced to, in the neighborhood of every point of a caustic of a general Lagrangian mapping in spaces with dimensions ≤ 4 . Along with the normal forms of functions we give the generating functions corresponding to large caustics in spaces with dimensions 3 and 4:

$$F(x,\lambda), \quad x \in \mathbb{R}^k, \quad \lambda \in \mathbb{R}^l, \quad k+l = n+1, \tag{2.64}$$

where n is the dimension of the Eulerian space. As usual, the caustic is defined as the set of critical values of the mapping

$$(x,\lambda) \mapsto (y,\lambda), \quad y_i = \frac{\partial F}{\partial x_i}$$
 (2.65)

and all normal forms of functions are acting in the neighborhood of the point 0.

2.6 Standard initial velocity fields in 2-dimensional space

In the previous section we shortly outlined the way of producing general transformations (metamorphoses) of caustics of Lagrangian mappings that connect the Lagrangian coordinate x of a particle with its Eulerian coordinate y at the time moment t. It was shown that an one-parameter family of Lagrangian mappings corresponds to the gradient motion of particles.

Let us consider now how to obtain the standard picture of motion of particles based on the theory of Lagrangian mappings. The idea of obtaining the general metamorphoses of instantaneous caustics was that the temporal evolution was considered as an Lagrangian mapping between spaces with dimensions higher by one compared to the initial Lagrangian or Eulerian spaces. This space corresponds to the space-time of the initial spaces. Consequently the large mapping gives us a whole picture of evolution. To clarify the principal questions of dynamical evolution of caustics and their transformations under violent relaxation, we consider first the dynamics in 2-dimensional space. In this case there are no problems of deciphering the results of modeling: it is possible to follow visually both the velocity and density fields. Here we derive the initial velocity fields for all types of metamorphoses of caustics (the birth of structures) in 2-dimensional space.

As the types of caustics and their transforms do not depend on a concrete form of the Hamiltonian, then for studying the general gravitational motion in 2-dimensional space, we can use the normal forms of Lagrangian mappings onto a 3-dimensional space that were derived in the previous section, based on the picture of the free motion of particles. Introduction of gravitation will not change the gradient nature of the mappings, the only change would be a monotonous relabeling of the time coordinate. The situation would change if the initial velocities were rotational, but it is well known that rotational modes in initial cosmological velocity fields decrease fast and practically disappear for the recombination moment, when the evolution of structure really begins. From the given list we see that the general caustics of this mapping do not have singularities, different from the cusps A_3 and the point-type singularities of three types: the swallowtail A_4 , the pyramid D_4^- and the purse D_4^+ (Fig. 2.1).

The isochrone is the level surface of the time function, defined in the 3dimensional Eulerian space-time. With change of time this surface moves also. The instantaneous caustic is obtained from the intersection of the large caustic with the isochrone. The change of the geometry of a caustic happens at that time moment when the isochrone touches the cuspidal line



Figure 2.1: General caustics of Langrangean mappings in 3-dimensional space: a) $- \operatorname{cusp}$, b) $- \operatorname{swallowtail}$, c) $- \operatorname{pyramid}$ and d) $- \operatorname{purse}$

of the large caustic or when it passes through one of the point singularities listed above.

The motion of particles is given by the motion of particles on a iso-chrone, that is the instantaneous Eulerian space with the coordinate system (y_1, y_2) . Let us consider an individual point with the Lagrangian coordinates $x = (x_1, x_2)$. If we replace the function of time in the normal form of the large mapping, then at every time moment this mapping maps the point x_1, x_2 to y_1, y_2 on this isochrone. This gives us the motion of the medium that corresponds to the current Lagrangian mapping. Caustics describe now the singularities of the density distribution of matter.

Generating functions and the function of time are defined locally around the 0-point of space-time. Thus in the following we study the motion of particles in a square with the side d < 1, the center of what coincides with the origin of coordinates y_1, y_2 . For modelling the formation of structure we suppose that in this square there are no singularities at the initial time. This will be equivalent to an initially homogeneous density distribution. This condition determines the initial time t_c , when the singularity appears, but at $t < t_c$, there are no singularities in the square. Recall that before bifurcation of a caustic the time t < 0, but after that t > 0; the bifurcation of a caustic happens at the time moment t = 0. We have to find this initial time moment for every type of bifurcation separately; for this it is necessary to study the geometry of caustics.

Let us begin with the bifurcation of type A_3 . The large mapping $(x, \lambda_1, \tau_1) \mapsto (y, \lambda_1, \tau_1)$ is determined according to the normal form $F(x, \lambda_1, \tau_1) = x^4 + \lambda_1 x^2$ as

$$y = \frac{\partial F}{\partial x} = 4x^3 + 2\lambda_1 x. \tag{2.66}$$

The critical set in the Lagrangian space (x, λ_1) is obtained from the equation

$$\frac{\partial y}{\partial x} = 12x^2 + 2\lambda_1 = 0, \quad \Longrightarrow x = \pm \sqrt{-\frac{\lambda_1}{6}}.$$
 (2.67)

The set of critical values (the large caustic) is obtained by substituting this equation into the definition of the Lagrangian mapping (2.66)

$$y = \pm 8 \left(-\frac{\lambda_1}{6} \right)^{3/2} \tag{2.68}$$

The large caustic in the space (y, λ_1, τ_1) is a half-cubic parabola on every plane $\tau_1 = const$ (Fig. 2.2). Along the coordinate axis τ_1 lie the points of type A_3 , forming the so-called cuspidal edge. The surface that is joining to this line consists of points of type A_2 (Morse points). The remaining space is filled with non-critical values of the large mapping. From Table 2.1 one can see that there exist five different types of isochrones. The isochrone $t = \tau_1$ determines a plane parallel to the coordinate plane y, λ_1). Temporal caustics are formed by the section of the large caustic with the isochrone. In this case there is no bifurcation. At every time moment the caustic has the form of a half-cubic parabola with the edge passing through zero and there is no time moment when the density at the zero point is regular.

In the second time function $t = \pm \lambda_1 \pm \tau_1^2$ there are four different combinations of signs. As a result we obtain two opposite oriented parabola, moving in different directions in the 3-dimensional space (y, λ_1, τ_1) . As the time function does not depend on the coordinate y, so for clarity we can consider these parabola in the plane (λ_1, τ_1) (Fig. 2.2. From the figure it is clear how the sections between the isochrone and the large caustic look like, and this gives metamorphoses of caustics of the series A_3 (Figure 2.3. As we see, for bifurcations of the series $A_3(-, -), A_3(+, +)$ and $A_3(+, -)$ there exists a moment t_c , when there is no caustic in the square with the edge d around zero in the plane (y, τ_1) . The bifurcation of type $A_3(-, +)$



Figure 2.2: Intersections of the isochrone with the plane (λ_1, τ_1) at different times t < 0, t = 0 and t > 0, corresponding to different time functions of bifurcation A_3 : a) $-t = -\lambda_1 - \tau_1^2$, b) $-t = \lambda_1 + \tau_1^2$, c) $-t = \lambda_1 - \tau_1^2$ and d) $-t = -\lambda_1 + \tau_1^2$.

(the so-called 2-dimensional analog of the "pancake birth" in the theory of Zel'dovich) does not have any singularities at t < 0. We find the initial time t_c for the type $A_3(-, -)$ from the condition, that the coordinate τ_1 of the edge (the cuspidal point) at this moment is equal to d/2 (Fig. 2.3(a)). Let us use the equation that defines the critical set (2.67):

$$6x^2 + \lambda_1 = 0. (2.69)$$

The edge moves along the line y = 0. Using this, we obtain from (2.66) an equation for the coordinate x:

$$4x^2 + 2\lambda_1 x = 0. (2.70)$$

This equation has a solution

$$x_1 = 0, \quad x_2 = \sqrt{-\frac{\lambda_1}{2}}.$$
 (2.71)

Both solutions, substituted into equation (6.4), give

$$\lambda_1 = -t - \tau_1^2 = 0. \tag{2.72}$$

This gives us the equation of motion of the cuspidal point of the caustic

$$\tau_1 = \pm \sqrt{-t}, \quad \Longrightarrow t_c = -\frac{d^2}{4}.$$
 (2.73)

If $t < t_c$, there is no caustic in the square.



Figure 2.3: Bifurcations of instantaneous caustics of type A_3 , obtained using different time functions: a) – the metamorphose of caustics of type $A_3(-, -)$, b) – $A_3(+, +)$, c) – $A_3(+, -)$ and d) – $A_3(-, +)$ (creation of a pancake in 2-dimensional space). We show the square of size d where there are no singularities at the initial time t_c .

For the bifurcation $A_3(+,+)$ we obtain the time t_c from the contact condition of the caustic with the square at the point y = d/2, $\tau = 0$ (Fig. 2.3b). The equation (2.68) that defines the large caustic gives us

$$\frac{d}{2} = \pm 8 \left(-\frac{\lambda_1}{6} \right)^{3/2}.$$
 (2.74)

After substituting here the time function $t = \lambda_1 + \tau_1^2$ at $\tau_1 = 0$, we obtain

$$d = \pm 16 \left(-\frac{t_c}{6} \right)^{3/2}.$$
 (2.75)

and the time is determined by

$$t_c = -6 \left(\frac{d}{16}\right)^{2/3}.$$
 (2.76)

Let us find the time t_c for the bifurcation $A_3(+, -)$. The caustic touches the square now at its corners (Fig. 2.3(c)). We choose the corner with the coordinates $\tau_1 = y = d/2$. From the equation of the large caustic (2.68), after substitution of $t = \lambda_1 - \tau_1^2$, we obtain for the plane (y, τ_1) the equation of the instantaneous caustic

$$y = \pm 8 \left(-\frac{t + \tau_1^2}{6} \right)^{3/2}.$$
 (2.77)

Substituting into (2.77) the contact condition $y = \tau_1 = d/2$, we obtain

$$t_c = -6\left(\frac{d}{16}\right)^{2/3} - \frac{d^2}{4}.$$
 (2.78)

The Lagrangian sub-space (x_1, x_2) labels different points in the Eulerian space (y_1, y_2) . From this follows the definition of velocity in the Eulerian space:

$$\begin{aligned} v_{y_1} &= \left. \frac{\partial y_1}{\partial t} \right|_{x_1, x_2}, \\ v_{y_2} &= \left. \frac{\partial y_2}{\partial t} \right|_{x_1, x_2}. \end{aligned}$$
 (2.79)

With the substitution of the function of time into the normal form of the large mapping, we obtain the equation of motion of a particle with the Lagrangian coordinates (x_1, x_2)

$$y_1 = f_1(x_1, x_2; t), \quad y_2 = f_2(x_1, x_2; t).$$
 (2.80)

Recall that now there is no natural relation between the Lagrangian and Eulerian coordinates,

$$x_1 = y_1|_{t=t_0}, \quad x_2 = y_2|_{t=t_0}.$$
 (2.81)

because the large mapping $(x,t) \mapsto (y,t)$ is a general family of functions, but the property of the Lagrangian space – labeling of different points – is held.

Currently, the Lagrangian space consists of coordinates (x, τ_1) and the Eulerian of (y, τ_1) . Thus in the direction of τ_1 the particles do not move. The equations of motion for all types of bifurcation of the series A_3 are given by

$$A_{3}(-,-): y = 4x^{3} - 2(t + \tau_{1}^{2})x, \quad v_{y} = -2x,$$

$$A_{3}(+,+): y = 4x^{3} + 2(t - \tau_{1}^{2})x, \quad v_{y} = 2x$$

$$A_{3}(+,-): y = 4x^{3} + 2(t + \tau_{1}^{2})x, \quad v_{y} = 2x,$$

$$A_{3}(-,+): y = 4x^{3} - 2(t - \tau_{1}^{2})x, \quad v_{y} = -2x.$$

(2.82)

To find the velocities at the point (y, τ_1) of the Eulerian space at the moment $t < t_c$, it is necessary to find the corresponding coordinates x in the Lagrangian space using the equation of motion (2.82) and to replace them in the expression for velocities in (2.82).

The singularities of the series A have the co-rank 1. This means the degeneracy of the critical point in one direction. That is why the corresponding vector field is zero in one direction (that of the degenerate coordinate).

Let us study now the large caustic A_4 , the so-called swallowtail. According to the normal form the large mapping can be expressed as

$$y = \frac{\partial F}{\partial x} = 5x^4 + 3\lambda_1 x^2 + 2\lambda_2 x. \tag{2.83}$$

The caustic consists of the surface of critical values of the mapping of type A_2 : in this surface there are lines of points A_3 and the point A_4 (Fig. 2.1). The bifurcation happens when then isochrone $t = \pm \lambda_1$ passes through the critical point A_4 .

At the points A_2 the derivative of the mapping equals to zero, thus the critical set can be determined by the equation

$$20x^3 + 6\lambda_1 x + 2\lambda_2 = 0. (2.84)$$

The time function is equal to the coordinate λ_1 (up to the sign), thus the instantaneous critical sets are situated in the planes (x, λ_2) and they can be described by the function $\lambda_2 = -10x^3 \pm 3tx$. This function passes through the origin of coordinates at any time t. The mapping $(x, \lambda_2) \mapsto (y, \lambda_2)$ that is defined by the normal form of the large mapping at every time moment, does not move the origin of coordinates. Consequently, at any time t the curve, consisting of the critical values of a mapping of type A_2 ,

passes through the origin of coordinates of the plane (y, λ_2) and there does not exist an initial moment t_c , when there are no singularities at some neighborhood of the zero point. This means that the bifurcation of type A_4 does not enter our list of transforms of caustics in 2-dimensional space, because we are interested in the initial velocity fields that correspond to a smooth initial density of particles.

Transformations of the caustic A_4 can be used for studying the evolution of an already formed singularity of type A_2 . This topic, however, does not fit into the limits of the current work. (Recall that we are dealing with oifurcations of caustics in 2-dimensional space. In 3-dimensional space the bifurcations can be different.)

It remains to study bifurcations of a caustic of type D_4 in 2-dimensional space. At a critical point D_4 the Hessian of the germ of the Lagrangian mapping has a co-rank 2. Consequently the family of Lagrangian mappings can be expressed in the form of the projection of a surface, depending on parameters, onto a plane. This projection is defined by the generating function (Table 2.1) of the large mapping $(x_1, x_2, \lambda_1) \mapsto (y_1, y_2, \lambda_1)$ in the following way:

$$y_1 = \frac{\partial F}{\partial x_1}, \quad y_2 = \frac{\partial F}{\partial x_2}.$$
 (2.85)

In case of D_4 , there are two non-equivalent normal forms D_4^- and D_4^+ . Geometrically this difference means that the large caustic D_4^- (the so-called pyramid) has three lines of singularities consisting of points of type A_3 , but D_4^+ has one cuspoidal edge (Fig. 2.1). These lines are passing through the point D_4^{\pm} . When the isochrone passes through this point, metamorphosis of the instantaneous caustic occurs.

Let us begin with the large caustic D_4^- in the 3-dimensional Eulerian space (y_1, y_2, λ_1) . The large mapping is defined by

$$y_1 = 6x_1x_2 + 6\lambda_1x_1,$$

$$y_2 = 3x_1^2 - 3x_2^2 + 6\lambda_1x_2.$$
(2.86)

We can find the critical set of points of type A_2 in the Lagrangian spacetime (x_1, x_2, λ_1) from the condition of degeneracy of the Hessian

$$det\left(\frac{\partial^2 F}{\partial x_i \partial x_j}\right) = 36(\lambda_1^2 - x_1^2 - x_2^2) = 0.$$
(2.87)

So the critical set is defined by the equation

$$x_1^2 + x_2^2 = \lambda_1^2 \tag{2.88}$$

that describes a two-sheet conic. Let us introduce the change of coordinates

$$\begin{aligned} x_1 &= \lambda_1 \cos \phi, \\ x_2 &= \lambda_1 \sin \phi. \end{aligned} \tag{2.89}$$

The equation of the critical set is satisfied, so with the substitution (2.89) into the equation of the large mapping (2.86) we obtain the equations that define the large caustic in the space (y_1, y_2, λ_1) :

$$y_1 = 3\lambda_1^2 f_1(\phi), y_2 = 3\lambda_1^2 f_2(\phi),$$
(2.90)

where

$$f_1(\phi) = \sin(2\phi) + 2\cos(\phi), f_2(\phi) = \cos(2\phi) + 2\sin(\phi).$$
(2.91)

As we see the caustic is symmetric relative to the plane (y_1, y_2) (Fig. 2.1). At a fixed λ_1 , the section of the caustic with a plane parallel to the coordinate plane (y_1, y_2) gives a closed curve that is determined by the dependence of the coordinates y_1, y_2 on ϕ . This curve consists of the critical values of type A_2 and has singularities of type A_3 (cuspoidal points). To find the positions of these singular points we differentiate the relations defining the caustic (2.90) by ϕ and assign to the derivatives zero values:

$$\frac{\partial y_1}{\partial \phi} = 3\lambda_1^2 (2\cos 2\phi - 2\sin \phi) = 0,$$

$$\frac{\partial y_2}{\partial \phi} = 3\lambda_1^2 (-2\sin 2\phi + 2\cos \phi) = 0.$$
 (2.92)

This system of equations will be satisfied in case of three values of $\phi = \phi_* : \pi/6, 5\pi/6$ and $3\pi/2$. The asimuthal coordinate ϕ in the Lagrangian plane (x_1, x_2) is connected to the corresponding coordinate in the Eulerian plane (y_1, y_2) by the relation

$$\tan \theta = \frac{y_2}{y_1} = \frac{f_2(\phi)}{f_1(\phi)}.$$
 (2.93)

It is possible to verify, by substitution, that for $\theta_* = \theta(\phi_*)$ the same values are obtained. So, for these angles the cuspoidal points are situated on the curve that was obtained by intersection of the large caustic with a plane, parallel to the coordinate plane (y_1, y_2) . In addition to that, the function $y_2(\phi)$ has an extremum at $\phi = \pi/2$.

We find the instantaneous caustic from the section of the isochrone with the large caustic. The form of the time function $t = -\lambda_1 + y_1 + ay_2$ suggests that the isochrone is a plane, tilted relative to the coordinate planes. We get the equation of the instantaneous caustic in the coordinates (y_1, y_2) after substituting the function of time in the equation of the large caustic (2.90).

$$y_1 = 3(-t + y_1 + ay_2)^2 f_1(\phi),$$

$$y_2 = 3(-t + y_1 + ay_2)^2 f_2(\phi),$$
(2.94)

Evaluating y_2 by y_1 using equation (2.93), one can solve the system (2.94) relative to $y_1(\phi), y_2(\phi)$. The obtained curve resembles a distorted triangle, with points A_3 at the corners (Fig. 2.4). Differentiating $y_1(\phi)$ and $y_2(\phi)$ we find that the singularities of these functions are situated at the same angles $\theta_* = \pi/6, 5\pi/6$ and $3\pi/2$ and at $\theta_* = \pi/2$. The curve $y_1(\phi), y_2(\phi)$) has the minimal value on the axis y_2 .



Figure 2.4: An instantaneous caustic of type D_4^- at time t < 0. In the square of size d there are no singularities.

To find the initial time t_c when the instantaneous caustic have not entered the square with the edge d, it is necessary to consider the points of the caustic that correspond to the values of asimuth $\theta = \pi/2, 5\pi/4, 7\pi/4$. In the coordinates y_1, y_2 the conditions of tangency with the square can be expressed as

$$\theta = \frac{\pi}{2}$$
: $y_1 = 0, \quad y_2 = \frac{d}{2},$ (2.95)

$$\theta = \frac{5\pi}{2}$$
: $y_1 = -\frac{d}{2}$, $y_2 = -\frac{d}{2}$, (2.96)

$$\theta = \frac{7\pi}{2}$$
: $y_1 = \frac{d}{2}$, $y_2 = -\frac{d}{2}$. (2.97)

From (2.95) and (2.94) we get that

$$\frac{d}{2} = 3\left(-t + a\frac{d}{2}\right)f_2(\phi).$$
(2.98)

As was said above, at the extremal points of $f_1(\phi)$ and $f_2(\phi)$, both asimuth coordinates ϕ and θ coincide. Thus, from (2.91) we find that $f_2(\pi/2) = 1$. At last we obtain

$$t_c = a \frac{d}{2} - \sqrt{\frac{d}{2}}.$$
 (2.99)

We choose the negative sign before the square root, because before bifurcation t < 0. In case of a highly inclined isochrone, the condition of the non-existence of a caustic in the square at t < 0 can be satisfied only for a rather small value of d. From the condition (2.96) $y_1 = y_2$, and from (2.93) we see that $f_1(\phi) = f_2(\phi) = f$, from which one can find ϕ at $\theta = 5\pi/4$, thus determining f. From (2.94) we obtain

$$t_c = -\frac{d}{2} - a\frac{d}{2} - \sqrt{\frac{d}{6f}}, \quad f = 1.073.$$
 (2.100)

By analogy, from condition (2.97) $f_1(\phi) = -f_2(\phi) = g$, from where we obtain g. From (2.94) it follows that

$$t_c = \frac{d}{2} - a\frac{d}{2} - \sqrt{\frac{d}{6g}}, \quad g = 0.735.$$
 (2.101)

From the obtained values t_c it is necessary to choose the smallest value for the current d and a. It is clear that the time given by equation (2.99) is the largest among these found for any d and a. Thus it is enough to consider only the formulae (2.100) and (2.101). For example, for d = 0.2 and a = 1, from (2.100) we obtain $t_c = -0.38$, but from (2.101) we find that $t_c = -0.21$. We choose the first value, because the caustic touches the lower left corner of the square ($\theta = 5\pi/4$) earlier than the right one ($\theta = 7\pi/4$).

The velocity field corresponding to the bifurcation D_4^- can be found using (2.79). Substituting in the function of time the coordinates y_1, y_2 by expressions (2.86) that define the Lagrangian mapping

$$t = -\lambda_1 + 6x_1x_2 + 6\lambda_1x_1 + 3ax_1^2 - 3ax_2^2 + 6a\lambda_1x_2 =$$

= $\lambda_1(-1 + 6x_1 + 6ax_2) + 6x_1x_2 + 3a(x_1^2 - x_2^2),$ (2.102)

we find

$$\lambda_1 = \frac{t - 6x_1x_2 - 3a(x_1^2 - x_2^2)}{-1 + 6x_1 + 6ax_2}.$$
(2.103)

Substituting (2.103) in (2.86) we obtain the dependence of the Eulerian coordinates on time

$$y_{1} = 6x_{1}x_{2} + 6x_{1}\frac{t - 6x_{1}x_{2} - 3a(x_{1}^{2} - x_{2}^{2})}{-1 + 6x_{1} + 6ax_{2}},$$

$$y_{2} = 3x_{1}^{2} - 3x_{2}^{2} + 6x_{2}\frac{t - 6x_{1}x_{2} - 3a(x_{1}^{2} - x_{2}^{2})}{-1 + 6x_{1} + 6ax_{2}}$$
(2.104)

and the required velocity field

$$v_{y_1} = \frac{6x_1}{-1 + 6x_1 + 6ax_2},$$

$$v_{y_1} = \frac{6x_2}{-1 + 6x_1 + 6ax_2}.$$
(2.105)

Establishing the dependencies of $x_1(y_1, y_2)$ and $x_2(y_1, y_2)$ at the initial time t_c , we obtain the initial velocity field in the Eulerian space.

We obtain the large mapping of type D_4^- from the generating function $F = 3x_1^2x_2 + x_2^3 + 3\lambda_1(x_1^2 - x_2^2)$ in the form

$$y_1 = 6x_1x_2 + 6\lambda_1x_1,$$

$$y_2 = 3x_1^2 + 3x_2^2 - 6\lambda_1x_2.$$
(2.106)

The critical set of points A_2 in the Lagrangian space-time is defined by

$$det\left(\frac{\partial^2 F}{\partial x_i \partial x_j}\right) = 36(x_2^2 - \lambda_1^2 - x_1^2) = 0 \qquad (2.107)$$

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$$x_2^2 = x_1^2 + \lambda_1^2. \tag{2.108}$$

Here the surface is a two-sheet conic with the rotation axis along the coordinate axis x_2 . Let us make a change of coordinates to satisfy the equation

$$\begin{aligned} x_1 &= \lambda_1 \sinh\phi, \\ x_2 &= \pm \lambda_1 \cosh\phi. \end{aligned} \tag{2.109}$$

The sign "+" corresponds to the conic in the half-space $x_2 > 0$, but the sign "-" gives the conic in the half-space $x_2 < 0$.

Substituting (2.109) into (2.106) we get the equations that determine the large caustic in the Eulearian space-time (y_1, y_2, λ_1)

$$y_1 = 3\lambda_1^2 f_1(\phi),$$

$$y_2 = 3\lambda_1^2 f_2(\phi),$$
(2.110)

where

$$f_1(\phi) = \pm \sinh 2\phi + 2\sinh \phi,$$

$$f_1(\phi) = \pm \sinh 2\phi + 2\sinh \phi.$$
(2.111)

This caustic consists of two surfaces, corresponding to the different conics in the critical set (Fig. 2.1). These surfaces intersect each other at $\lambda_1 = 0$. As seen from (2.110) the large caustic is symmetric relative to λ_1 . Intersection of the large caustic with the plane $\lambda_1 = 0$ gives us two curves. Let us find the extremal points of these curves relative to the coordinate axis y_1, y_2 . Let us consider first the curve corresponding to the sign "+":

$$\frac{\partial y_1}{\partial \phi} = 3\lambda^2 (2\cosh 2\phi + 2\cosh \phi) = 0,$$

$$\frac{\partial y_2}{\partial \phi} = 3\lambda^2 (2\sinh 2\phi - 2\sinh \phi) = 0.$$
 (2.112)

The first equation does not have a solution, because $\cosh \phi > 0$ at any ϕ . The second equation has a solution at $\phi = 0$.

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The connection between the asimuthal coordinate ϕ in the Lagrangian plane (x_1, x_2) and the corresponding angle θ in the Eulerian plane (y_1, y_2) is defined by

$$\tan \theta = \frac{y_2}{y_1} = \frac{f_2(\phi)}{f_1(\phi)} = \frac{\cosh 2\phi - 2\cosh \phi}{\sinh 2\phi - 2\sinh \phi}.$$
 (2.113)

At $\phi = 0$ we get $\theta = 3\pi/2$. This point is non-singular, because the derivative $\partial y_2/\partial y_1$ is finite (zero).

For the second curve, corresponding to the "-" sign in (2.109), we obtain the equations

$$\frac{\partial y_1}{\partial \phi} = 3\lambda_1^2 (-2\cosh 2\phi + 2\cosh \phi) = 0,$$

$$\frac{\partial y_2}{\partial \phi} = 3\lambda_1^2 (2\sinh 2\phi - 2\sinh \phi) = 0,$$
 (2.114)

This sytem has a solution $\phi = 0$. We find the Eulerian coordinate θ from the relation

$$\tan \theta = \frac{\cosh 2\phi + 2\cosh \phi}{-\sinh 2\phi + 2\sinh \phi},\tag{2.115}$$

that gives $\theta = \pi/2$. This coordinate corresponds to a singular point on the curve, because the derivative $\partial y_2/\partial y_1$ is undefined. This is a singularity of type A_3 . This means that on the large caustic there is a line of points A_3 that lies in the plane (y_2, λ_1) (Fig. 2.1).

The instantaneous caustic on the isochrone is obtained from the intersection of the large caustic with the isochrone that is defined by the function of time $t = \lambda_1 + y_1 + ay_2$ as a plane in the Eulerian space-time (y_1, y_2, λ_1) . After substituing the function of time into equations (2.110) that define the large caustic, we obtain the equations of the instantaneous caustic on a isochrone with the coordinates y_1, y_2 :

$$y_1 = 3(t - y_1 - ay_2)^2 f_1(\phi),$$

$$y_2 = 3(t - y_1 - ay_2)^2 f_2(\phi).$$
(2.116)

By analogy with case of D_4^- one can show that the extremal points of the curve of the instantaneous caustic are situated on the instantaneous caustic at the same angles θ as the plane $\lambda_1 = const$. Thus the cuspoidal point from one curve and the extremal point from another curve of caustic are lying on the y_2 -axis (Fig. 2.5). As time passes these two lines are approaching. At the moment of bifurcation t = 0 the isochrone passes through the point D_4^+



Figure 2.5: An instantaneous caustic of type D_4^+ at time t < 0. In the square of size d there are no singularities.

of the large caustic that is at the origin of coordinates. The instantaneous caustic looks like two curves emerging from the origin of coordinates at this moment.

We find the initial time t_c using the same methodology as in case of bifurcation D_4^- . The points of possible touching of the caustic with the square coincide with the points that are defined by formulas (2.95, 2.96, 2.97).

In case of (2.95) the square touches the cuspoidal point. From (2.116) and (2.95) we get the equation (at $\theta = \pi/2, \phi = 0$)

$$\frac{d}{2} = 3\left(t_c - a\frac{d}{2}\right)^2 f_2(0), \qquad (2.117)$$

where by (6.42)

$$f_2(0) = 3. (2.118)$$

From this

$$t_c = a\frac{d}{2} - \sqrt{\frac{d}{18}}.$$
 (2.119)

The remaining conditions (2.96) and (2.97) correspond to the lower curve (Fig. 2.5), for which the dependence on ϕ is given by

$$f_1(\phi) = \sinh 2\phi + 2\sinh\phi,$$

$$f_1(\phi) = \cosh 2\phi - 2\cosh\phi.$$
(2.120)

From (2.96) we obtain $f_1(\phi) = f_2(\phi) = f$. Now we can find ϕ in case of $\theta = 5\pi/4$ and with this determine f. We find for this corner of the square from (2.116) that

$$t_c = -\frac{d}{2} - a\frac{d}{2} - \sqrt{\frac{d}{6f}}, \quad f = 0.863.$$
 (2.121)

By analogy we find the appropriate ϕ from the equality $f_1(\phi) = f_2(\phi) = g$ together with the condition (2.97) and compute g. The time t_c is determined as

$$t_c = \frac{d}{2} - a\frac{d}{2} - \sqrt{\frac{d}{6g}}, \quad g = 0.863.$$
 (2.122)

These formulas are similar to (2.99, 2.100, 2.101), with the only difference in the values of f and g. The functions of time differ by the sign before λ_1 , but in both cases we choose isochrones with negative values of t.

Here the functions f and g are equal, so t_c is defined by (6.50b). The standard values d = 0.2 and a = 1 give $t_c = -0.40$.

Let us find now the distribution of velocities by equations (2.79). We change the coordinates y_1, y_2 in the function of time in accord with the Lagrangian mapping (2.106)

$$t = \lambda_1 + 6x_1x_2 + 6\lambda_1x_1 + 3ax_1^2 + 3ax_2^2 - 6\lambda_1ax_2.$$
(2.123)

From this we find

$$\lambda_1 = \frac{t - 6x_1x_2 - 3a(x_1^2 + x_2^2)}{1 + 6x_1 - 6ax_2}.$$
 (2.124)

We use this equation for the replacement of λ_1 in (2.106). As a result we get the equations of motion $y_i = f_i(x, t)$, where

$$y_{1} = 6x_{1}x_{2} + 6x_{1}\frac{t - 6x_{1}x_{2} - 3a(x_{1}^{2} + x_{2}^{2})}{1 + 6x_{1} - 6ax_{2}},$$

$$y_{2} = 3x_{1}^{2} + 3x_{2}^{2} - 6x_{2}\frac{t - 6x_{1}x_{2} - 3a(x_{1}^{2} + x_{2}^{2})}{1 + 6x_{1} - 6ax_{2}}.$$
(2.125)

From the definition of velocities (2.79) we find

$$v_{y_1} = \frac{6x_1}{1 + 6x_1 - 6ax_2},$$

$$v_{y_2} = \frac{6x_2}{1 + 6x_1 - 6ax_2}.$$
(2.126)

In order to find the initial distribution of velocities in the Eulerian space we determine for any point (y_1, y_2) the corresponding Lagrangian coordinates (x_1, x_2) at the time t_c by (2.125) and substitute these into (2.126). With this the list of general bifurcations of caustics in the 2-dimensional Eulerian space is exhausted. Using equations (2.79), (2.105) and (2.126) one can find the initial distribution of velocities at the moment t_c , when the Lagrangian mapping is one-to-one (does not have singularities) in the square $(-d/2, d/2) \times (-d/2, d/2)$ of the Eulerian plane (y_1, y_2) . In Figs. 2.6 and 2.7 we show the kinematical pictures of evolution of singularities of the series D_4 . These pictures were obtained as follows.

Consider particles on a homogenous grid in y_1, y_2 . Using equations (2.104) and (2.125) we find the corresponding Lagrangian coordinates x_1, x_2 at the moment t_c . Substituting them into equations (2.105), (2.126) we find the velocity of a particle with the coordinates y_1, y_2 at the initial time. The evolution of the particle distribution with time is desribed by the equations of inertial motion

$$y_i(t) = y_i(t_c) + tv_{y_i}, i = 1, 2.$$
(2.127)

In Figs. 2.6 and 2.7 we have given the positions and the velocities of the particles and the positions of the caustics at different times. The figures are spoiled somewhat by the boundaries of the initial square, because the velocities of points near the boundaries are non-zero.

2.7 Conclusions

We have determined standard initial velocity fields for the study of the dynamics of superclusters of galaxies. The theoretical base of the current work was the theory of Lagrangian mappings and a closely connected to it catastrophe theory. That is why we had to introduce shortly the basic notions and results of the above mentioned theories.

The theory of Lagrangian mappings allows us to study the general potential flows of continuous matter. From it follows the classification of general bifurcations of singularities of the matter distribution. In a realistic situation more complicated distributions of density could form, but the theory of Lagrangian mappings states that the singularities of density are geometrically equivalent to the caustics of a general Lagrangian mapping. This theory is local, even in time, thus the motion of interacting particles is similar to the motion of non-interacting particles during a small time interval. This is true until the formation of a density singularity, because it is not clear if the Lagrangian surfaces remain Lagrangian after this. There is hope that interaction between particles will change little the topology of caustics and their metamorphoses. To investigate this question one can use the "clean" initial conditions, found in this work for 2-dimensional space, and to numerically model the evolution of self-gravitating matter. Following the evolution of singularities of density it is possible to answer the question how the interaction influences the geometry of caustics.

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Figure 2.6: Metamorphoses of caustics of the type D_4^- at the moments 1) t=-0.43, 2) t=-0.04, 3) t=0 and 4) t=0.04; a) instantaneous caustic, b) distribution of particles and c) distribution of velocities. To demonstrate better the evolution of the particle density, the region occupied by particles is enlarged up to the initial dimensions.



Figure 2.7: Metamorphoses of caustics of the type D_4^+ at times 1) t=-0.40, 2) t=-0.04, 3) t=0 and 4) t=0.04; a) instantaneous caustic, b) distribution of particles and c) distribution of velocities. The scaling is chosen as in Fig. 2.6.

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Chapter 3

Multigrid versus FFT methods for simulating gravitational collapse

3.1 Introduction

Investigation of self-gravitating systems requires solving the Poisson equation for each time step. Usually in numerical solutions of this problem a discrete analog of the Poisson equation is solved by using the Fast Fourier Tranoform (FFT). Existence of effective FFT algo- rithms (Hockney 1970, McClellan *et al.* 1979) makes its use very cheap and popular.

Nevertheless, numerical simulations have serious limitations, due to limited power and storage capacity of present-day computers. Recent cosmological computer models deal up to 10^6 particles and have 64 grid- points per spatial direction. As one can see (Bouchet 1985) this spatial resolution is not enough to handle correctly nonlinear evolution of gravitating systems in smaller scales. There are two main error sources in such simulations. One is due to a limited computing precision (truncation error) and another is due to a discrete nature of models (grid effects). As known, FFT algorithms work on homogeneous grids where the spatial meshsize is fixed. To obtain larger resolution one must introduce finer discretization to the whole computing volume. In multi-dimensional problems this approach is often unacceptable.

An alternative way to solve the Poisson equation is the Multigrid (MG) method. This method is widely used in fluid dynamics, but we know only one case of its use in astrophysical computations (Tacharnuter 1979). The main advantages of the MG algorithm are a) smoothing, of high frequency errors (minimizing thus truncation errors) and b) ability to work with grids of arbitrary size and discretization types. The last property enables its to develope adaptive MG algorithms in which the local grid refinement depends on the smoothness of the solution. Thus one can obtain, In prin-

ciple, a solution which better approximates the exact analytical soluti- tion.

The main purpose of this paper is to compare two solvers of the Poisson equation, one based on the FFT and another - an the MG method. Firstly we briefly describe the basic principles of the MG algorithm used. The second section describes the analytical solution for a test problem. Generating initial conditions according to this problem we ran two series of simulations, with different potential solvers. The results are presented in the third section.

3.2 Test problem

For simplicity we chose an one-dimensional collapse of an isolated system with an initially uniform density (a box-like density distribution). For such a system the equations of motion are satisfied by a self-similar solution:

$$\boldsymbol{x}(t) = \boldsymbol{a}(t)\boldsymbol{x}_0 \tag{3.1}$$

where $x_0 = x(O)$ is the initial coordinate of a particle. The density ρ remains uniform during the collapse, only its value changes:

$$\rho(t) = \left| \frac{\partial x_0}{\partial x} \right| = \frac{\rho_0}{|a(t)|},\tag{3.2}$$

where $\rho_0 = \rho(O)$.

From the one-dimensional Poisson equation

$$\frac{\partial^2 \phi}{\partial x^2} = \rho \tag{3.3}$$

we see that inside the system the acceleration depends linearly on the coordinate

$$\frac{d^2x}{dt^2} = -\frac{\partial\phi}{\partial x} = -\rho(t)x. \tag{3.4}$$

Using (3.1) and (3.2) we get an equation for the scale function a(t)

$$\frac{d^2a}{dt^2} = -\rho_0 \frac{a}{|a|}.$$
 (3.5)

Up to the time T of the first collapse the scale function a(t) > 0. Using an initial conditions a(O) = 1 and $\dot{a}(O) = O$ (zero initial velocities) we find the solution

$$a(t) = 1 - \frac{\rho_0 t^2}{2}.$$
(3.6)

The collapse time T can be found from the condition a(T) = O:

$$T = \sqrt{2/\rho_0}.\tag{3.7}$$

At this moment all points pass through the centre of the system x = 0and, consequently, the density is infinite. But the acceleration remains finite and only its sign changes. So afterwards the system evolves exactly as before collapse. only In the reverse direction. At a time 2T the system returns to the initial size, density and velocity distributions. Thus in the continuous limit our collisionless model will pulsate with a period of 2T(4T for any particle).

An one can see this analytical model includes some nonphysical properties which are hard to follow in computer simulations. Particularly it concerns the discontinuities of the density distribution at the boundary points, and infinite density at the moments of collapse. The last is not so drastic for dynamics because the acceleration remains finite.

In the analytical model there to no evidence of the dynamical relaxation in the system, due to special Initial conditions. From a physical point of view the density must remain finite so at the moments of collapse the system cannot behave according to the analytic solution. Accounting for inevitable numerical errors one may expect some dynamical relaxation to start in the computer model. Various algorithms can be now ranked according to the period of smooth evolution (up to onset of relaxation).

3.3 Multigrid method

Multigrid (MG) methods give rather flexible algorithms for solving partial differential equations. During the past decade they were theoretically explored and developed further (Brandt 1977, Dold *et al.*1982). The approach is sufficiently general so it can be used for solving nonlinear problems and even integro-differential equations.

In this article the MG method is described as used in the present work. More information on advanced MG techniques can be found in the papers mentioned above. We start with a set of uniform grids with decreasing mesh-sizes $h_0 > h_1 > \cdots > h_M$ where the mesh-size ratio $h_{k+1} : h_k = 1 : 2$. On each gridlevel G^k one can define an usual difference equation of the form

$$L^{k}U^{k}(x) = F^{k}(x), \qquad (3.8)$$

where the L^k in our case are the difference analogues of the Laplace operator.

The main idea of the MG method is to use the solution on the coarser grid as the correction to the solution on the current level. More specifically, let u^k be an approximate solution of the G^k problem, and let

$$L^k u^k = F^k - f^k. aga{3.9}$$

The exact discrete solution is $U^k = u^k + v^k$, where the correction v^k satisfies the residual equations

$$L^k v^k = f^k. aga{3.10}$$

It is evident that not every G^k problem has a meaningful approximation on a coarser grid G^{k-1} . For instance, if the residual f^k fluctuates rapidly on G^k , with wavelength less than $4h_k$, these fluctuations are not visible on, and therefore cannot he approximated by the coarser grid.

An effective way to damp rapid fluctuations in residuals is to use relaxation procedures, e.g. the Gauss-Seidel relaxation. It uses the discrete equations for the initial problem. Particularly, if we are interested in solving the one-dimensional Poisson equation, the usual second-order discretization can he written as

$$\frac{U_{i+1}^k - 2U_i^k + U_{i-1}^k}{h_k^2} = F_i^k, \tag{3.11}$$

where

$$U_i^k = U^k(ih_k), F_i^k = F^k(ih_k).$$

In the Gauss-Seidel relaxation the points of G^k are scanned one by one in some prescribed order (we used left to right scanning). At each point the value u_i is replaced by a new value u_i^* , such that Eq.(3.4) at that point is satisfied. That is, u_i^* satisfies

$$\frac{u_{i+1} - 2u_i^* + u_{i-1}}{h_k^2} = F_i^k, \qquad (3.12)$$

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where the new value u_{i-1}^* has been computed at a previous spatial step.

For the first few iterations such procedures usually converge well, with residuals rapidly decreasing from one iteration to the next, but soon afterwards the convergence rate levels off and becomes very slow. Closer examination shows that the convergence is fast as long as the residuals have strong fluctuations on the scale of the grid. So this is the point where relaxation sweeps should be discontinued and an approximate solution of the (smoothed out) residual equations by coarser grids should be employed.

So the MG iteration an level k to obtain the next approximation of u_k consist of the following steps:

a) Choose $v_k = u_k$ and $d_k = f_k$, as a first approximation for the residual functions.

b) Smooth v_k applying m_1 relaxation sweeps.

c) Transfer the defect to the next coarser grid:

$$d_{k-1} - I_k^{k-1}(d_k - L_k v_k),$$

where I_k^{k-1} is the fine-to-coarse transfer operator. If the level is not the coarsest then go to step b).

d) Solve exactly the equation $L_0v_0 = d_0$. For the coarsest grid this is inexpensive.

a) Interpolate the correction to the next finer grid and compute the corrected approximation:

$$v_{k+1} = v_{k+1} + I_k^{k+1} v_k.$$

f) Smooth v_k applying m_2 relaxation sweeps.

g) If we have returned to the initial level, then the new approximation is $u_k = v_k$, else goto to step e).

In our computer program we used for the fine to coarse transfer the simple injection of grid-function values at middle points. The coarse- to-fine transfer was accomplished by a bilinear interpolation. For the coarsest level we solved the appropriate difference equations exactly, using the Gauss-Jordan method.

To start the MG iteration at the finest level one can choose $u_M = 0$ as a first approximation and proceed as described above. Boundary conditions are implicitly accounted for in this scheme during the transfers between grid levels. If they include values of derivatives at boundaries, they must be relaxed also.

The next step toward improved efficiency is to use the full multigrid (FMG) technique. It is also an iterative procedure and it's idea is to use a coarser discretization level as a good initial approximation for the iteration

on the next (finer) level. The realization of the FMG algorithm is shown by the next flow chart.

a)Start on the coarsest level k = 0. Solve exactly $L_0 u_0 = f_0$

b) Transfer the solution to a finer level using an interpolation of second (or higher) degree.

c) Apply r times the MG iteration on this level as described above.

e) If the current level is not the finest then return to step b), otherwise you have obtained the final FMG solution of $L_M u_M = f_M$.

It seems that there is a fair lot of work to do in computing the MG solution. But as theoretical predictions and applications show it is not too large. This is mainly due to an effective use of the multigrid idea in conduction with effective error damping smoothers. Programming of the MG algorithm is also quite simple. For example, our implementation of FMG consists of about 200 lines of C-code.

3.4 Comparison of two methods

The goal of this work was to compare to alternative methods of solving the Poisson equation: one based on the FFT and another on the MG algorithm. For this purpose two programs were developed, differing only in the potential solvers.

As known, FFT is based on periodic functions and consequently the mass distribution repeats itself with a certain spatial period. To consider effectively isolated gravitating systems (as prescribed by our test problem) one must use FFT on a domain which well exceeds the scale of the system. This must be done to decrease the influence of neighbouring systems on the central one. Further, if we center the gravitating mass with respect to the computing domain then we must use cosine functions in the Fourier expansion and respectively the cosine transform to solve the Poisson equation.

In the MG algorithm there are no predefined basic functions so this method is better suited to treat isolated systems. For the boundary conditions we simply choose the potential to he zero at the boundary points.

The Poisson equation was discretized using the two-point Laplacian difference scheme. The FFT potential solver is based on the Winograd's star-algorithm [12]. Theoretical predictions argue that the number of algebraic operations (multiplications) are reduced to the theoretical minimum in this method. Compared with usual FFT algorithms (including FACR) the number of multiplications is 3-10 times smaller. Another feature of the Winograd's algorithm is that the number of meshpoints is not a power of two but it may obtained by multiplying quantities which, have no com-

mon factors. For example we used two grids with N=16*7*3=336 and N=16*9*3=1008.

The MG algorithm was used with the finest grid consisting of N=113 meshpoints (including two boundary points). As one can see, in the FFT computations 3 and 9 time larger meshes were used to diminish the influence of neighbours to the dynamics of the system. We chose five gridlevels, so the coarsest level consisted of $(N-1)/2^{k-1} = 7$ meshpoints.

During the computation it was enough to use only one FMG iteration to obtain the residual norm below 10^{-5} .

As said, we started from a box-like density profile where the mass is distributed uniformly in the range l = (N/2 - 28, N/2 + 28), where N is the number of meshpoints. For this we put one masspoint at every mesh point in l (57 points total). In this case the computation of density according to the CIC scheme gives us the density distribution at the boundary points consistent with the analytic model. Obviously in the case of one point per cell one must expect quite large density fluc- tuations to develop at grid points which may affect the dynamical behaviour of the system. To investigate this possibility we made series of FFT and MG experiments with ten points per cell. To obtain the same time scale the density was accordingly normalized. When there is more points per cell the CIC scheme does not produce a box-like density profile. Consequently the dynamics at boundary points differs from the analytic solution as shown below.

The integration in time was carried out using the leap-frog scheme. The initial timestep was 0.01 and it was divided by two every time when the maximal displacement of points was over 0.25. The energy conservation between timesteps was better than 0.2as in the standard CIC scheme , which is widely used In cosmological N-body models.

In total we carried out three FFT and two CIC experiments. The main parameters of the FFT experiments were as follows: 1) the number of gridpoints N=336, the number of masspoints n=57 (denoted by FFT336-57), 2) N=336, n=570 (FFT336-570) and 3) N=1008, n=57 (FFT1008-57). The MG, computations were carried out with 1) N=113, n=57 (MG113-97) and 2) N=113, n=570 (MG113-570).

According to the analytical solution our system must pulsate with a period of 2T, where the collapse time T is given by (3.7). Initially $\rho_0 = 1$ so $T = \sqrt{2}$. We followed the evolution of the system up to t = 10.0 so it is expected to pulsate through five periods.

During the computation we traced the changes of the central density. This gave us the first collapse time of our models. In the following table there are listed collapse times t_C obtained in different experiments along
Table 3.1: Collapse Times.

Experiment	t_C	Deviation
FFT336-57	1.525	7.83
FFT336-570	1.525	7.83
FFT1008-57	1.450	2.53
MG113-57	1.415	0.06
MG113-570	1.420	0.41

with deviations from the theoretical times.



Figure 3.1: Boundary velocity in different models.

As one can see, the MG models gave values which are very close to the theoretical one. In the FFT experiments the collapse time depends on the mesh length. As was expected, better consistency is obtained in the FFT1008-57 experiment where the grid-length is larger and consequently the influence of neighbouring periods is smaller. Comparing with the MG experiments we added four empty spatial periods to both sides of the initial computing period (N=112). From the value of the collapse time we can conclude that even this is not enough to exactly simulate an iso- lated system.

In Fig. 3.1 we demonstrate the behaviour of the velocity at the system's leftmost point. As seen, the velocities in the FFT experiments deviate more from the theoretical curves than MG ones. This can he also explained by the fact that in the FFT computations the model is not exactly isolated. Another conclusion that can be drawn from Fig. 3.1 is that the growth of the number of points per cell makes the consistency with the theoretical model worse. As was pointed out earlier this may be caused by the wrong density behaviour near the system boundaries due to the CIC scheme. With a trapezium-like density distribution the forces at boundary points are smaller compared with the case of hatbox density distribution.

In Figs. 3.2, 3.3 and 3.4 we demonstrate the the evolution of force and den- sity in FFT1008-57 and MG113-57 experiments. As was expected, the current test is fairly hard for numerical simulation. The main troubles are the discontinuities of density and force at boundary points, and it is difficult to retain the linearity of the force versus distance.

The FFT method solves theoretically exactly the discrete Poisson equation because the Fourier harmonics are the eigenfunctions of the discrete Laplacian. But if one takes into account the computing errors (truncation errors) then obviously in the FFT transform they accumulate, producing high frequency components in the solution. In the MG method there exists a high frequency smoother which effectly damps the influence of truncation errors and expectedly produces a better solution to the differential equations. From the Figs. 3.2, 3.3 and 3.4 one can see that in the MG experiment the force and density profiles are smoother and the discontinituties are conserved for a longer time.

However, the uniformity of the density and the linearity of the force are eventually violated. As seen from Figs. 3.2 and 3.3 of density evolution there arise density fluctuations at gridpoints which later increase. We suppose that this is mainly due to discretisation errors with a scale of some meshizes. The main source of these errors is the CIC scheme of computing density and force. To overcome this one may use better resolution.

So the discretisation of the initial smooth problem distorts its dynamics, and we can see from Figs. 3.2, 3.3 and 3.4 that typical violent relaxation occurs in the system. But the FFT transform adds through computing errors more secondary maximums than occur in corresponding, MG experiments. So in this case the MG algorithm works better than the FFT.

Of great interest to users is the effectiveness of both methods, the main descriptive parameters being the memory requirements and speed. The

storage required for the MG algorithm is only a fraction more than the number of locations, say, 2N, required to store the potential and density values on the finest grid. Indeed, for a *d*-dimensional problem, a storage of roughly $2N/2^d$ locations is required to store those values on next coarser grid. and so on. The total for all levels is

$$2N(1+2^{-d}+2^{-2d}+\cdot) = 2N\frac{2^d}{2^d-1}.$$
(3.13)

In advanced MG schemes there exist methods of a major reduction of storage. To compare the speed of two alternative methods we computed 1000 times the potential for a grid of 113 points and find that the FFT spent for this 172 seconds and the MG solver — 270 seconds. It is a fairly good ratio compared with the work done in the MG algorithm, and with better results. For isolated systems the FFT solver needs larger gridsize and there it will work even slower than the MG solver.

3.5 Conclusions

In this paper a multigrid method to numerically solve of the Poisson equation was described and used. We compared this method with the FFT solver for a simple model with a known analytical solution, which describes the special case of homogeneous one-dimensional collapse. Theoretically this system does not relax, it only pulsates with a fixed period. From a physical point of view, however some relaxation may be expected.

Numerical models show that relaxation occurs but it is hard to extract real relaxation from the artificial one, due to computing errors. However, the multigrid method used here has properties, which make its use preferable compared with the FFT. The multigrid method is better suited for studing isolated systems and it includes a high frequency error smoother which effectively damps truncation errors. Thus it seems to be a better method to use for simulating gravitational dynamics.

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Figure 3.2: Density evolution in a) MG113-57 and b) FFT1008-57(cont.)



Figure 3.3: Density evolution in a) MG113-57 and b) FFT1008-57



Figure 3.4: Acceleration evolution in a) MG113-57 and b) FFT1008-57.

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Chapter 4

An adaptive multigrid solver for high-resolution cosmological simulations

4.1 Introduction

It is common knowledge that the dynamical and spatial resolution of standard cosmological simulations of smooth (dark) matter evolution is rather low. The basic particle-mesh (PM) code smooths the density on a grid and finds the potential using FFT-type techniques. As shown by Bouchet, Adam & Pellat (1985), grid effects damp the growth of structure for all scales smaller than at least 6 cell sizes. This restricts considerably the range of scales where we can believe our models.

In order to improve the situation several different methods have been proposed. The best known of them is the PPPM (particle-particle particlemesh) code, developed by Eastwood & Hockney (1974) and described in detail in their book (Hockney & Eastwood 1981). It finds the large-scale forces from the smoothed density, as does the basic PM code, but uses the nearby mass points to calculate the detailed short-range force. This code was adapted for cosmological simulations by Efstathiou *et al.*(1985), and is presently the standard code for cosmology. Couchman (1991) has modified it for situations where the density range becomes large and most of the time in the PPPM code would be spent on calculating pair interactions, introducing adaptive mesh refinement in order to reduce the amount of calculations of pairwise forces.

The ultimate high-resolution code is the tree code, proposed by Barnes & Hut (1986) and first used for cosmological simulations by Bouchet & Hernquist (1988). This code treates all interactions between gravitating masses basically on a pairwise basis and is thus free from any grid effects.

Both the PPPM code and the tree code are based on the paradigm of individual clouds of matter. Although a softened force is usually used, it is not clear how well the massive clouds represent the essentially continuous distribution of dark matter. Thus it is necessary to develop a high-resolution code for this class of problems.

The first of such codes, a multiple mesh particle code, was proposed by Chan *et al.*(1986), who use local higher resolution grid patches in highdensity regions. Another mesh refinement method has been proposed by Villumsen (1989). These methods differ mainly in their approach to solving field equations on local grids. Chan *et al.*(1986) obtain the local grid potential as a solution to a boundary value problem for the Poisson equation on the local grid, where the boundary values are defined from the solution on a global coarser grid. They find the solution on local grids by an efficient iterative scheme. Villumsen (1989) considers the local potential as a sum of a solution for the distribution of matter on the subgrid, using isolated boundary conditions, and the external global solution for the full matter distribution (without the mass at refined regions). He uses FFT to find the potentials, and special tricks to speed up the solution for the isolated local patches.

As we see, in the latter approach there is no backreaction from submesh particles to the global grid; the coarser periodical part of the field is computed without subgrid particles. In the Chan *et al.* method this backreaction is included.

An important issue intrinsic to all multiple resolution mesh schemes is how well they treat particles that enter subgrids. In principle, when switching to a higher resolution, force anisotropies and radial errors should be less than those on a coarser grid, and additional errors will be generated mainly by solution errors near grid interfaces. In the case of a boundary value problem (the Chan *et al.* approach), the error depends on interpolation errors on the boundary and on the density estimate at the grid point next to the boundary. For the Villumsen code the errors are generated by an external lower resolution solution from a coarser grid and by the density estimation both at the grid boundary and at neighbouring grid points.

In the Couchman's AP^3M code that uses force splitting to long-range and short-range parts (intrinsic to P^3M), the mesh part of the force is approximated by a smooth reference interparticle force $R(r, a_m)$, where a_m is the softening scale appropriate for the current mesh resolution. The potential is calculated using a modified Greens function which minimizes the differences between computed and reference forces. The total mesh part of the force acting on a particle is found by summing the force $R(r, a_m)$ from the base (periodical) mesh and the forces due to particles on a refinement, calculated with a different softening scale a_s , and the system is locally considered as isolated.

The main difference between the Chan *et al.*, Villumsen and Couchman codes is that in the former two the aim of the mesh refinement is to enhance the resolution of the force field through a higher resolution potential field, whilst in the last code the refined grid is introduced mainly to reduce the computational overhead in the short-range force calculation in the case of heavy clustering of particles. A smaller gridsize allows us to use a smaller neighbouring radius r_c , reducing the number of particles that need to be used for the short-range force correction. Another advantage of AP^3M is the adaptive dynamic creation of submeshes.

This paper presents another adaptive algorithm for a continuous density distribution, based on the well-known multigrid method (Brandt 1977). We shall give a short overview of the method below. The main positive features of the multigrid method are that for the case of the Poisson equation its computational complexity scales with number of grid-points N as O(N), it allows one to control the errors inherent in the solution of the Poisson equation, and it lends itself naturally to adaptive refinement. It is also very flexible in applying different boundary conditions and allowing special treatment if necessary.

Compared with the methods described above, our implementation of the adaptive multigrid solver for the Poisson equation is physically closest to that of Chan et al., as it finds the local grid potential as the solution for the boundary value problem defined by a coarser grid solution. The main difference is that in the adaptive multigrid method the creation of subgrids is a natural part of the solution process. The local refinements are introduced during multigrid iteration in locations where predefined error estimates demand it. There is a tight dependence between the coarse grid solution and a finer grid solution, as the coarse grid is used for correction of the solution on the finer grid and vice versa. At the internal boundaries (subgrid interfaces) the values of the potential change during the search for an overall solution, due to changes in the finer grid solution. This is natural, because they should agree despite the different scales of the discretization and interpolation errors. The point is that the local grid problem should be solved together with the global problem. If we treat it separately, we contradict the global boundary conditions. The natural boundary conditions for the local problem are the Dirichlet conditions, as these guarantee that the potential will be continuous at subgrid boundaries.

Comparison of our approach with the Couchman code is not straightforward, due to the different approaches of the force calculation. In AP^3M the global (periodic) part of the potential is calculated coarsely and the local (non-periodic) part is found using isolated boundary conditions, so there is no backreaction to large scales. However, as the force resolution is enhanced further using local direct summation, the backreaction effects may be less important.

Our code has already been applied to the modelling of gravitational microlensing (Schramm *et al.*1991). We describe here its application to cosmological situations, and follow as an example the birth and the subsequent evolution of a typical pancake singularity.

4.2 Multigrid description

Multigrid methods were introduced for solving boundary value problems by Brandt (1977). Quite comprehensive reviews of multigrid methods can be found in Press *et al.* (1992) and Brandt (1984).

As the name implies, in this method the problem is solved iteratively, using several sets of grids with different fineness. In the standard case the mesh size ratio of the grids at neighbouring levels H/h = 2, where H is the coarser grid mesh size, and the points of the coarser grid coincide with every second point of the finer grid. The solutions on the coarser grids are used to estimate the smooth components of the final solution and the increasingly finer grids are used to determine details of the solution. We refer readers to the recent introduction in Press et al. (1992, section 19.6) and will not give the details of the multigrid method here, noting only that we use the Full Multigrid algorithm (FMG), the Gauss-Seidel red-black relaxation to smooth the high-frequency error components, and the Full Approximation Storage (FAS) algorithm in order to be able to introduce finer grid levels adaptively.

In standard multigrid problems the source term (r.h.s. of the equations) is usually well determined. In gravitational simulations, however, the density distribution is sampled by discrete mass points, and the problem of determining the matter density on different grid levels is rather complicated. We shall describe our approach below.

We start with a fixed number of levels of uniform grids G_h which cover all the computing domain. On the finest level we compute the density D_h from particles using the cloud-in-cell (CIC) algorithm in the chosen computational volume and make a linked list of particles inside the volume. At the end of the density computation we also find the boundary values of the potential field f_h using this density. In this way we have defined the r.h.s. term of our differential equation for a grid with mesh size h:

$$\mathcal{L}_h F_h = D_h,$$

subject to the boundary condition

$$F_h = f_h,$$

on the boundary of G_h , where \mathcal{L}_h is in our case the usual 7-point finite difference operator for the Laplace equation.

Having solved this equation approximately on the level G_h , using coarser levels to accelerate the solution process, we proceed by adaptively introducing finer grid levels. We have used the value of the local density as the criterion for deciding if there is a need for finer grids, but there are other possibilities. One of the most popular criteria used is the local truncation error (the difference between the discrete $\mathcal{L}_h F_h$ and the analytical $\mathcal{L}F$) which is a natural byproduct of any multigrid solution. To apply the local density criteria we mark during the density computation the gridpoints where the density is higher than a chosen threshold. By analysing this flag field we define the flag clusters that could be bounded by rectangular grid boxes. As we use at present only non-overlapping grids, some postprocessing is necessary.

After allocating new grids, we compute the density on these grids using the particle lists from the coarser level that contains the current grid. We also create a new point list for this particular grid, consisting of those points only that are inside the grid, and we subtract this list from the pointlist of the coarser grid in order to keep points divided between grids. First, this eliminates unnecessary scans over the full particle array, and, secondly, these lists are needed later on if we start to move particles around on our collection of grids.

Besides the density, we interpolate the boundary values for the potential from those on the coarse grid in order to specify the local Dirichlet problem. We repeat the multigrid solution process on new grids using coarser grids and generating new finer grids until the desired resolution is achieved. For every iteration we update the density on coarser levels by the fine level density in order to keep our differential equation consistent on different grid levels. It is possible to use the CIC scheme for density computation, but, as the cells at different grid levels cover different volumes, the density estimates differ for the same point at different levels. This introduces additional noise which makes the convergence more difficult. Thus one has either to introduce spatial averaging for coarser grids or to invent a density measure which gives the same value at the same point in space independent of the mesh size of a grid. In the present code we have used the full weighting scheme which finds densities on coarser grids by averaging densities over neighbouring points on the finer grid.

The multigrid solution process stops after making a few additional iterations on the finest level and checking that the changes in the solution are less than the truncation error norm on that level times a small factor (usually 0.01). This ensures that the discrete solution is solved down to truncation errors. Usually it takes 3-5 multigrid iterations to get the solution to a desired accuracy. Compared to 'exact' solvers, such as for example FFT, multigrid is an O(N) procedure, only the multiplicative factor in this estimate could be larger. Nevertheless, multigrid is quite comparable in speed to FFT (Foerster & Witsch 1982) for medium N and could be more efficient for large N. There exist several versions of parallel multigrid codes (e.g. Tuminaro 1989; and Gärtel *et al.*1991).

We compare the exact (r^{-2}) force-radius law with that obtained by the multigrid code in Fig. 4.1. The figure shows the averaged pairwise force between a massive particle and massless test particles which were homogeneously distributed in logarithmic radial bins and randomly in angular coordinates. The massive particles were randomly distributed on the finest subgrid. The force was computed using the usual second-order differencing scheme. The curve labelled TH gives the exact force for point particles; the curve labelled MG is the usual smooth-field force which has to go to zero for zero radius in order to avoid self-forces for a (CIC) particle. The curve labelled AMG is the result of an adaptive refinement by two levels - as we divide the mesh size by 2 for the next finest grid, this curve is shifted to factor of 4 smaller coordinate values, as it should be. We have shown also the rms relative radial and tangential force fluctuations which are around 0.1 per cent of the adaptive mesh force. The maximum deviations from the mean mesh force that we found in our experiments were around 10 per cent, but their population was extremely small (only a few cases from an average of about 15000 points per radial bin). These deviations arose at the boundaries of subgrids and are typical for the single massive point case; similar deviations should not occur in the case of a continuous density distribution.

Special care has to be taken with calculation of forces near boundaries of adaptive refinements. As was mentioned above, the boundary values of the potential for local fine grids are obtained by interpolation from the coarser grid. This guarantees the continuity of the solution across the boundary. but not necessarily the continuity of its derivative (force). To smooth possible jumps in force estimates on boundaries of subgrids, we found these

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Figure 4.1: The forces obtained from the multigrid simulation compared to the exact r^{-2} force, versus distance (in grid cell units). The force scale is given as a decimal logarithm, but the distance is given as a base two logarithm. The exact force (labelled TH) is shown by a solid line, the basic mean multigrid force (MG) by a dashed line, and the mean force obtained from a two-level finer adaptive solution (AMG) by a dotted line. The two latter forces were found by choosing randomly the position of a massive point and then calculating forces at a number of positions around it. The lines labelled RF and TF show the rms relative radial and tangential force fluctuations with respect to the mean radial force (AMG) obtained with adaptive grids.

forces also by interpolation from the coarser grid. (We used cubic interpolation if there were enough data points, otherwise linear interpolation was used.) As grids are simply a mathematical artefact, particles should not feel the crossing over between grids of different resolution. Our procedure enables particles to change grids smoothly.

Apart from the multigrid Poisson equation solver, other parts of our code are similar to those in the usual PM code. We move particles with a standard leapfrog integrator (we change the timestep, though) on every grid, where the particles are taken from the point list that belongs to that grid. The time step is controlled by the Courant condition: the maximum change of a coordinate should be less than a fraction of the mesh size (we have used one-half). We can have different masses for particles, and for our cosmological sphere we can guarantee mass conservation by reflecting the exiting particles back from the opposite side. The code is not too large: the main modules add up to about 6200 lines of C programming language.

4.3 Testing the code

The code we developed first is meant to be used for studying the evolution of generic types of density singularities. There are only a few of these, all listed in Arnold (1980), and they can be thought of as typical progenitors of large-scale structure, describing the regions of the first collapse. On scales where there has not yet been any significant interaction of neighbouring elements of structure (superclusters), the models of singularities can describe the actual dynamics and geometry of structure.

In order to understand the evolution of specific singularities we have to study first the case of isolated singularities, using vacuum boundary conditions. In order to minimize the influence of the geometry of the computational volume on the results, we have to work in a sphere. Of course, working in a cube would be much simpler, but we have not been able to get rid of the ghosts of the cube in the final configurations.

Use of isolated boundary conditions on a sphere might seem to be contrary to the usual cosmological practice of periodic boundary conditions. In the case of the treecode, where vacuum boundaries arise naturally, people have taken enough trouble to modify the code to mimic periodic boundaries better (Bouchet & Hernquist 1988; Hernquist, Bouchet & Suto 1991). Thus we have to check if our isolated region models the evolution of structure in cosmology well enough.

As there are really no perfect numerical methods to use for comparison, one should use the exact solutions for the evolution of structure. There are only three of these — one for the linear regime and two non-linear solutions, one for a spherical top-hat collapse and the other for a one-dimensional plane wave. The latter solution clearly cannot be used in our case, so only two remain.

We use the usual cosmological equations for the evolution of structure for the $\Omega = 1$ universe in comoving coordinates x, connected with the physical coordinates r by r = a(t) x, where a(t) is the scale factor that describes the expansion of the universe. We choose this function as the new time coordinate, and write our basic equations as

$$\Delta \Phi = \delta, \tag{4.1}$$

where Φ is a suitably normalized gravitational potential and δ is the usual

density contrast, and

$$\frac{du}{da} + \frac{3}{2a}u = -\frac{3}{2a^2}\nabla\Phi,\tag{4.2}$$

where u = dx/da. Our equations are similar to those used by Matarrese et al.(1992).

In order to test for linear evolution, we have to generate appropriate initial data — a realization of a Gaussian random field with a given power spectrum. One starts usually with the power spectrum of the density contrast:

$$P(k) = < | ilde{\delta}(k)|^2 >_{|k|=k},$$

where k are the wavenumbers and $\tilde{\delta}$ are the Fourier amplitudes of the density contrast. We proceed by following the method described by Nusser & Dekel (1990).

In the linear approximation the movement of particles can be described by the formula derived by Zeldovich (1970):

$$x = q + a u(q), \tag{4.3}$$

where q are the initial (Lagrangian) coordinates and the velocity u(q) depends on q only. This leads to the (linear) relation between density and velocity

$$\delta(q) = a \, \nabla_q \cdot u.$$

The latter relation can be satisfied if the Fourier amplitudes of the velocity are

$$\tilde{u}(k) = \frac{k}{k^2} \tilde{\delta}(k). \tag{4.4}$$

Having chosen the complex Fourier amplitudes for the density contrast A(k) + iB(k) as random Gaussian numbers with a distribution N(0, P(k)) on an appropriate grid k_i in wavenumber space $(-N/2 \le k_i \le N/2)$, where N is the resolution of the grid), we can form the Fourier amplitudes of the velocity by (4.4) and find the velocity field in real space by an inverse Fourier transform. We use the Fourier transform algorithm for real 3D data from Press *et al.* (1992).

For tests we used a low-resolution model, 28 cells for the diameter of a sphere (32 for the surrounding cube that we use to fix the boundary conditions), in order to see the influence of a discrete grid clearly in both methods. If we wish to get a good representation of small perturbations, the density has to be generated from a regular grid. We chose 8 particles per grid cell which made the total particle number rather large, 64^3 for the PM cube and about 100000 for the sphere.

For the initial density spectrum we chose white noise, in order to see better the damping of high-frequency modes. We generated the initial velocity field as described above, and generated the coordinate displacements from a regular q-grid, choosing them to be proportional to velocities and normalized to a fixed (small) rms displacement amplitude. As we work in a sphere, but the FFT works in rectangular regions, we first found the displacements in a 32^3 cube and then set the displacements outside our sphere to zero.



Figure 4.2: The ratio of the rms density contrast to the value expected from the linear theory, versus the scale factor a. The solid line is for the PM code; the dotted line is for the MG code.

We have to take a little more trouble about the velocities. As the highfrequency modes of the velocity that we generated cannot be caused (and changed) by the potential found from the same grid, our initial state is too hot. To remedy this we used the quiet start recipe proposed by Efstathiou et al. (1985). We recalculated the velocities, finding the density, solving for the potential and using the linear approximation relation between acceler-



Figure 4.3: The normalized rms velocity contrast (constant in the linear theory) versus the scale factor a. The solid line is for the PM code; the dotted line is for the MG code.

ation and velocity, which for our case $(\Omega = 1)$ reads:

$$u = \frac{1}{a} \nabla \Phi. \tag{4.5}$$

In the linear case we can check for the evolution of the velocity and density fields. If the initial velocities are given by the above formula, it is easy to see that the velocities have to remain constant, du/dt = 0, (see also (4.2)). The continuity equation

$$\frac{d\delta}{da} + (1+\delta)\nabla \cdot u = 0$$

tells us that the density contrast has to grow linearly with a.

We started from the rms amplitude 0.025 for the density contrast and followed the evolution of structure from a = 1 until a = 10. The results are not too good — see Figs 4.3 and 4.3. In Fig. 4.3 we show the ratio of our rms density contrast to the expected value from linear theory (the curve labelled MG). As is seen, the evolution lags behind the true rate and the difference reaches about a factor of 2.5 at the scale factor a = 10. A



Figure 4.4: The spectral dependence of the ratio of the amplitude of the density contrast at a = 10 to its theoretical value. The abscissae k are given in units of 1/L (the inverse cube size); the solid curve describes the PM-code and the dotted curve for the MG code.

similar picture can be seen in Fig. 4.3 – while the rms velocity is expected to remain constant, it actually drops in time (although the differences are smaller than these for the density).

This discrepancy is typical for smooth-field simulations, and is mainly caused by damping of high-frequency modes. Bouchet *et al.* (1985) have studied it extensively in the case of PM codes. Most of the reasons for the damping, the CIC density assignment scheme and a finite grid size, are present in our code too. In order to have standard errors to compare with, we solved the same problems by a standard PM code. There are, certainly, better codes around, but simple PM is a pure smooth-field algorithm, similar to multigrid, in contrast to improved PPPM-type codes. We used a 32^3 grid with periodic boundary conditions, and the same number of particles (8) per cell, and started from the same initial state. The corresponding curves in Figs 4.3 and 4.3 (labelled PM) look similar: the density contrast behaves a little better in the PM code, the velocity drops a little faster, but differences between the two codes are small.

We can understand what is happening a little better if we look at the

evolution of the density on different scales. In Fig. 4.4 we give the ratio of the density spectra at the epoch a = 10 to that at the start of the calculations, normalized by the theoretical growth factor. If we look at the PM code curve we see that the largest scales closely follow the linear growth law, but the difference comes in at smaller scales. The MG curve shows us that this damping is also present in multigrid, although to a lesser extent. As we calculated our spectra in a 32^3 cube, the largest wavelengths present in a cube do not fit into our sphere and we have a slight drop in the MG case for these scales, but otherwise the MG code with isolated boundary conditions describes the evolution of small perturbations at least as well as does the periodic PM code.

The second test we made is the highly non-linear spherical top-hat collapse. This is also a textbook problem which can be solved exactly (see, e.g., Padmanabhan 1993, section 8.2). We shall check for the moment of collapse a_{coll} which is predicted to be

$$a_{coll} = (\frac{3\pi}{2})^{2/3} \frac{a_i}{\delta_i},$$

where δ_i is the initial density contrast for the sphere (at the scale a_i) and the only approximation used to get this result is the requirement $\delta_i \ll 1$.

As the dependence of the collapse time on the initial density contrast is rather strong, one has to take care when generating the initial distribution. We generated, first, points on a regular mesh inside a sphere (with an initial grid of 28 cells per diameter), 8 points per cell, and left a hollow sphere inside, with a radius of 0.75 of that of the large sphere. We then filled this sphere also with points on a regular mesh, but with a slightly smaller mesh size. In order to compare the results we generated a similar sphere inside a 32^3 cube, with a radius of 0.75 of the half-cube size, and followed its evolution by our PM code. Although the central densities were the same in both cases, the initial mean densities and density contrasts were different (the cube had a larger volume) and the predicted collapse times differ also.

The boundary conditions were fixed (zero for zero total mass in a sphere) for the multigrid and periodic for the PM code. We estimated the moment of collapse by finding the moment of maximum density (the density dispersion peaked also at the same time). Fig. 4.5 shows the collapse history for both cases, expressed in terms of the normalized collapse time, a/a_{coll} . The simple multigrid solution (labelled MG) gives a slightly better result than the PM code, but they both lag behind the exact solution. This is due to the smoothing effect of a rather coarse grid. The PM peak is higher than the MG peak, as there is more mass in the collapsing sphere in the first case.



Figure 4.5: The evolution of the maximum density for a spherical cosmological collapse. The abscissae are given in units of the theoretical collapse time. PM denotes the particle-mesh code, MG the multigrid code and ADMG the adaptive multigrid code with two additional finer levels. The ADMG curve is scaled down (by a factor of 15.7) in order to see all curves together.

We solved the problem also with an adaptive multigrid code, going down two finer levels. Grids on a finer level were generated when the local density went higher than a chosen threshold (24 points per cell). The behaviour of the maximum density in this case is shown in Fig. 4.5 by the curve labelled ADMG. As we see, this gives us a result that is closer to the exact solution. In this case it is also rather difficult to estimate the theoretical time — the CIC scheme gives systematically higher densities in regions where some components of the density gradient are zero. This problem can be removed by additional smoothing, but we did not want to suffer an extra loss of resolution. Instead of this we built the initial CIC density histogram, found the mass in the central cell at the collapse and estimated the initial density contrast as an average over this mass.

The adaptive multigrid gets closer to the exact solution, and the density peak is much better determined here (the ADMG densities on the graph are divided by 15.7 to get them into the graph). We looked also at the density distributions, hoping to see differences, but these were small. This case allows us also to compare the relative speeds of the codes. On a SPARCstation-10/51 one timestep of the fully adaptive multigrid took 5.8 s (1.2 s for the calculation of density, 3.6 s for the potential, together with new density calculations at finer grid levels and 1 s to push the particles). One PM step took 4.7 s (0.8+0.3+2.3). As is seen, the time is mainly determined by the number of particles (106 944 for the multigrid sphere, 260 488 for the PM cube) and this makes them similar; also, the FFT solver is about ten times faster for this small grid size.

4.4 An application: a high-resolution 3D pancake

Careful inspection of published high-resolution cosmological simulations (in 2D, of course) indicates that there might be only a few specific types of elements of structure, and the higher the resolution is, the more intriguing become the repetitive structures on smaller and smaller scales. Of course, the observed supercluster chains and the knots they emerge from also look similar to some extent.

There is a mathematical basis for this similarity — if we agree that visible structure forms in locations of the highest density (for cold dark matter this means an infinite density), then we should look for possible classifications of density singularities. This has been, fortunately, already done, and the corresponding theory is called the theory of singularities of Lagrangian mappings. Matter flows in a gravitating medium follow Lagrangian mappings, so this theory is relevant to the formation of structure. This was realized at least ten years ago, and these mappings have been used in cosmology by Arnold, Shandarin & Zeldovich (1982). A very important point is that the number of different mappings in the generic case (the number of types of structure elements) is surprisingly small, only six in 3D space and four in 2D (Arnold 1980; Arnold 1983). If we look at the evolution of these singularities in time, we are dealing with a metamorphosis of the singularities, and there are from two to five types of evolution for every basic singularity type, which is a small number.

The singularity mappings describe the motion of matter only until flows intersect, and it is not clear how useful they are afterwards. And, as these mappings are local, we do not know how long they will remain so before being distorted by interaction with neighbouring singularities.

This all is a subject of fascinating study, and we can use the basic types of mappings to find the initial conditions for the emerging structures. As they are generic, these are the structures that must be most common both in the sky and in the simulations. The code that we can use to study the formation of structure clearly has to be as high-resolution as possible. This was the motivation for starting the development of the present code.

As usual in a new field, there is a mass of new problems and intricacies here. We shall demonstrate how our code works and shall describe these problems using the most familiar Lagrangian singularity — the Zeldovich pancake. It belongs to the so-called type A_3 , and the birth of a pancake is described by the metamorphosis $A_3(-,+)$.

This mapping can be described by the coordinate transformation (from Lagrangian coordinates to the normal Eulerian space)

$$\begin{aligned} x_1 &= 4q_1^3 + 2(q_2^2 + q_3^2 - t)q_1, \\ x_2 &= q_2, \\ x_3 &= q_3, \end{aligned}$$
 (4.6)

where x are the Eulerian and q the Lagrangian coordinates. This mapping is meant to be used near the zero-point of coordinates, that is, the place where the pancake is born — the density is

$$\rho(x(q)) = |\frac{\partial x}{\partial q}|^{-1} = |12q_1^2 + 2(q_2^2 + q_3^2 - t)|^{-1},$$

and, when time grows from $-\infty$ towards the future, this density first becomes infinite at t = 0 in x = 0.

The velocities for this mapping can also be found (Suisalu 1987):

$$v_1 = -2q_1,$$

 $v_2 = 0,$ (4.7)
 $v_3 = 0$ (4.8)

(all A-type singularities are essentially one-dimensional).

These formulae are in principle all that one needs to set up a pancake birth simulation. The remainder are technical details, but they are rather important. The main problem is that the mapping is non-linear, and, if we want to model it, we must restrict the mapping to a finite region a sphere is the best choice, as it minimally distorts the final results. The mappings (4.6) and (4.7) are free to change using any diffeomorphism we want, as this does not essentially change the mapping in the centre of the coordinates. However, if we want to study as large a region around the centre as possible, the modification must be minimal. Our choice is

$$x = f(q)(1 - q^2/R^2) + q q^2/R^2,$$
(4.9)

where f(q) is the mapping (4.6) and R is the radius of the sphere. The velocities are changed similarly:

$$v = w(q)(1 - q^2/R^2),$$
 (4.10)

where w(q) is the original (Eulerian) velocity in the Lagrangian coordinates (4.7). This is not a perfect solution, as it gives us a constant density and zero velocities on a Lagrangian sphere $q^2 = R^2$, and thus distorts the geometry of our Eulerian computational volume. We have fought this by choosing a small radius, R = 0.05, as the region inside it maps practically into an Eulerian sphere (our initial time parameter t = 0.4). For simulations we choose the scale factor a as the time variable. The times a and t can be connected to each other by any monotonic transformation. We are also at liberty to choose the velocity amplitude – this amounts to changing the time unit. We did this by using the quiet start recipe – we built the point distribution by the mapping (4.9), found the density (the maximum initial density contrast was 0.308), solved for the potential and used the linear evolution formula (4.5) to find the initial dynamical velocities. We used both the dynamical velocities and the velocities from the mapping scaled down to make the maximum velocities coincide in both cases.

The initial grid is the same as we used for the spherical collapse, a sphere with a diameter of 28 cells (in Lagrangian coordinates). In order to see the details of the structure better, we choosed 27 points per grid cell, distributed regularly, a total of 324 609 points. If the number of points per cell gets larger than 70 we create a finer rectangular subgrid with double the linear resolution. We have limited the number of refinement levels to five – this limit is imposed mostly by the noise that accumulates during the run. This means that the effective spatial resolution in the central subgrid is 1/1024. Also, in this case the boundary conditions will change in time – we found them by direct summation over the initial (32^3) grid. We used the same equations of motion as before, working in the $\Omega = 1$ cosmology.

We illustrate the results by a series of figures. As the results for the initial velocities from the mappings and from the dynamics did not differ much, we shall use the case of the mapping (truly unidirectional) velocities. The figures all refer to the time a = 13.6 (we started with a = 1). The first series of figures (Figs 4.6 (a)-(d)) shows the distribution of mass points in thin (one cell of the basic grid) slices along the x_1 - x_2 coordinate plane. We have also shown the borders of the subgrids, and the change of scale can be followed from the coordinate values.

As this is already a well-advanced state of collapse, we see a fairly rich substructure in the figures. Fig. 4.6 (a) covers the whole slice, and

the pancake is clearly seen in the centre. The edges of the pancake are formed by the turnback points of the first particle stream that has passed the pancake plane. Only four subgrids can be seen in this figure, the two smallest are too small. The lense-like overall geometry of the collapse is a generic property of this type of singularity and is determined by the mapping itself. It is possible to distort the shape a little, in principle, but we discovered that such a distortion will not last long — the mapping we used is generic.

Fig. 4.6 (b) (coinciding with the third subgrid) shows the central part of the collapsed region. We see two perpendicular planes and the formation of ellipsoidal shells – these are the turnback regions of smaller-scale flows, and the collapse tends to become more spherical. This differs from the picture seen in high-resolution 2D simulations by Beacom *et al.* (1991), and is probably caused by the fact that 3D gravitation is in general more effective than 2D gravitation. These shells cannot be caused by the spherical boundary: these flows have been developed in the centre where they do not feel the large-scale symmetry. Neither can they be the result of the growing temperature: this effect can be seen in the centre only (Fig. 4.6 (d)).

Fig. 4.6 (c) shows the central matter distribution in more detail – we see a much smaller pancake in the centre, with a size about 80 times smaller than that of the largest pancake. The last figure in this series, Fig. 4.6 (d), shows no more detail although the last grid has 13×17 cells in this plane. This is probably caused by the (numerical) heating during the collapse. The central density contrast is 1.6×110^5 ; this value can be taken to characterize the dynamical resolution of the simulation.

Figs 4.7 (a)-(d) show slices from the x_2 - x_3 plane, using similar scales to the previous series. In Fig. 4.7 (a) we see the whole plane, where the outer density enhancement is the edge of the main pancake. More inner density ridges can be seen in Fig. 4.7 (b). They are rather well resolved in Fig. 4.7 (c), and the central part can be seen as a small hot lens in Fig. 4.7 (d). The spokes along the coordinate axes that are evident in all these figures are caused either by the anisotropy of the 7-point difference operator, or by the CIC density assignment algorithm which gives enhanced densities along the coordinate planes and axes. These spokes are not too prominent, however.

In the last series of figures (Figs 4.8 (a)-(d)) we have tried to show the 3D density distribution. Each of these figures is a 3D representation of three density levels, cut in half by an x_1 - x_2 coordinate plane (in these figures the coordinate x_1 is vertical). The smaller inner cube in Figs. 4.8 (a)-(c) shows the size of the large cube in the next figure. The density



Figure 4.6: The central x_1 - x_2 slices of the simulation of the birth of a pancake $(A_3(-, +) \text{ metamorphosis})$ at the epoch a = 13.6. The simulation started at a = 1 with a maximum density contrast $\delta_{max} = 0.308$ and with the velocity amplitude found from linear dynamics. Panels (a)-(d) show the particle distribution in slices on different scales; the boxes show adaptive subgrids.



Figure 4.7: The central x_2 - x_3 slices of the same density distribution as in Fig. 4.9 Panels (a)-(d) show the particle distribution in a slice on different scales; the boxes show adaptive subgrids.



Figure 4.8: A three-dimensional representation of the same density distribution as in Figs. 4.6 and 4.7. A region of space between chosen density levels is cleared to show the inner density levels (see Table 4.1). Panels (a-d) show the density distribution in increasingly smaller scales - the small cube in the centre shows the size of the next panel.

panel	density level				
	outer	inner	central		
a	0.02	0.7	10.5		
b	14.4	33.5	173.3		
с	185.2	924.4	11090.0		
d	9244.0	46220.0	154000.0		

Table 4.1: Density levels in the 3D configuration.

values for the different level surfaces (the outer one, the inner surface of the 'shell' and the outer surface of the central feature) are given in Table 4.1. The surfaces are better seen in Fig. 4.8 (a), where the density resolution is 1/32 of the cube size. In Figs 4.8 (b)-(d) the resolution is 1/24 and is probably a little too low for the IDL(Interactive Data Language – a graphical software package from Research Inc.) shade-volume command to manage. Of course, in the real density distribution there are no holes: they are cut out in the figures only to help to visualize the continuous density distribution.

Fig. 4.8 (a) starts showing us the basic sphere and the primary pancake inside. The outer shell is, in fact, continuous, and looks striped by the IDL effects. Fig. 4.8 (b) shows a second pancake inside the first one (look at the sizing cubes) and a high-density detail at the centre. This detail is better resolved in Fig. 4.8 (c), showing a density enhancement that is oriented perpendicularly to the original pancake plane (there is a trace of it in Fig. 4.6 (b), the horizontal density enhancement). The plane itself also has rather high density here.

The central core of Fig. 4.8 (c) is resolved in Fig. 4.8 (d) — it is a lenselike density concentration along the original pancake plane (the vertical density enhancement in Fig. 4.6 (b)), and the small pancake of Fig. 4.6 (d) stays in its centre.

As is seen, the inner regions grow more and more irregular with decreasing scale and increasing density. This could be due to a number of reasons. The first of these is the numerical heating caused mainly by the force fluctuations at the edges of subgrids. Another is the fact that we have probably not taken proper care when arranging the initial mappings, and as a result these are not cool enough.

4.5 Conclusions

We have presented here an adaptive multigrid code for gravitational simulations and tested it for cosmological problems. The multigrid approach lends itself naturally to adaptive refinement and does not impose any restrictions on the boundary conditions to be used. It does not much use more memory than the popular cosmological codes and it is fast enough to be used on present computers.

The list of possible enhancements is rather long. We have already implemented the case of periodic boundary conditions which are more suitable to simulate the evolution of global structure. We are planning to use better difference operators in order to get more isotropic forces, and we have ideas on how to improve the density assignment algorithm. The speed of our algorithm is still lower than that of the FFT, but we can use the potential and grids from the previous time step to enhance the convergence — this can be done because we keep the potential separate from the density field. Probably the use of block time will also speed up the code. We determine our boundary conditions at present by direct summation over the grid we can either use a coarser grid for this or use an FFT solver. IS has also implemented the code on a parallel computer (2D case on a CM-200), but this implementation needs further work.

As for the present application of following the structure of singularities, this has shown us the importance of setting up clean initial conditions and getting rid of noise for truly high-resolution simulations. A typical example is the CIC density assignment scheme – the fact that it may give spurious density enhancements does not worry anybody as long as we are using noisy initial conditions, but in the present case its deficiencies were obvious.

Acknowledgments. This code has taken a long time to mature, and IS has worked on it, besides at his home institute Tartu Astrophysical Observatory, at ESO, at Cambridge, at MPI für Astrophysik, and longest at NORDITA, where this work was finished. ES spent a month at NORDITA to help to bring the code into the cosmological environment. We thank all these institutions for their hospitality and stimulating atmosphere. We also thank our referee, Dr H.M.P. Couchman, for his competent and useful advice.

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Chapter 5

Gravitational collisions in cosmological N-body codes

5.1 Introduction

Cosmological simulations use *N*-body algorithms that replace the initially continuous distribution of (dark) matter by discrete and rather massive 'particles'. This helps to simulate intersecting streams of collisionless matter that are common at the time of formation of cosmological structure. Interactions between these particles may, however, differ from the dynamics of the continuous media they are meant to approximate. The main source of discrepancies are close encounters between the particles (gravitational collisions).

The popular belief has been that if the number of points in the simulation is sufficiently large, the discreteness effects (gravitational collisions or close encounters between mass points) do not play an important role. These effects have been studied only for tree-codes in the case of stationary gravitating systems (Hernquist & Barnes 1990, Huang, Dubinski & Carlberg 1993). We shall describe in this paper the role of gravitational collisions in high-resolution cosmological codes.

Among the different N-body algorithms used for cosmological simulations the P^3M (Particle-Particle-Particle-Mesh) algorithm has become the industry standard for high-resolution simulations. It was designed initially for plasma physics simulations and ported to cosmology by Efstathiou & Eastwood (1981). It has been clearly documented in textbooks (Hockney & Eastwood, 1988, Couchman, 1995) and the code is practically in public domain. This code was the first candidate for our study.

The P^3M -code considerably improves the resolution of a standard PM (Particle-Mesh) code by splitting forces in two parts — the long-range force from the overall density distribution on a mesh and the short-range force

from nearest neighbours, calculating the latter by summation over pairs of particles. The algorithm was devised initially to simulate collections of pointlike particles. In cosmological simulations of formation of structure the basic dark matter density is smooth and does not lend itself easily to representation by discrete mass points. This difficulty is usually alleviated by introducing smoothing parameters in pairwise forces, effectively replacing the mass points by extended spherical clouds.

In order to study discreteness properties of the P^3M -code one should have smooth codes with spatial resolution comparable to the P^3M . Such codes have appeared only recently, and most of them are grid-based multiresolution schemes (except that of Pen (1994) that uses a global deformed grid). These codes improve the spatial resolution in selected regions (mostly in those of high density). We shall describe these codes and their main differences below; for comparison we used our adaptive multigrid code (Suisalu & Saar 1995).

We also ran one simulation using the popular tree-code (Barnes & Hut 1986). Its deflection properties have been studied before (Hernquist & Barnes 1990, Huang et al. 1993), but for a stationary case only.

The usual tool for measuring pairwise collisions is the study of energy diffusion (see the studies of three-code simulations cited above). This is proper for stationary gravitating systems, where energy is otherwise conserved and heating comes only from pairwise interactions; in cosmology the overall energy changes with time and it is not the best measure for collisions. We propose instead of it to study orbital deflection angles, concentrating only on the change of direction of velocities and not on the change of their absolute values.

5.2 Simulations

As the adaptive grid methods are not as well known as the P^3M and one is forced to select between different versions, we shall describe their differences below.

All these methods form subgrids of higher spatial resolution in regions where density is higher than a prescribed limit. They use for boundary conditions on a subgrid the values of the potential (Dirichlet conditions) interpolated from the coarser grid, but they differ in finding the solutions for the potential. The problem is if the coarse grid solution should depend on the finer grid solution at the same point, or not. It certainly should if we used exact direct solvers of linear systems arising from discretized partial differential equations, but the situation is not clear for approximate iterative solvers. In cosmological simulations we do not have an exact source term, either, as our density determination may depend on a grid level. In an ideal situation solutions of different resolution should converge

In an ideal situation solutions of different resolution should converge rapidly during the iteration process. In practice convergence is rather slow, as solutions on coarser grids are changed considerably by temporary solutions on finer subgrids (see, e.g. Brandt 1987). This issue has been discussed by Anninos, Norman & Clarke (1994) who classify adaptive grid methods as having either one or two-way interfaces between parent and subgrids.

As an example, in the multi-grid method developed by Jessop, Duncan & Smith (1994) only one-way grid interfaces are used that implies that the local fine grid solution can be different from the coarse grid solution. They find the local solution by iteration on the subgrid only. A recent adaptive code by Splinter (1995) uses a similar methodology, although the algorithms for finding the solution on subgrids differ. In contrast, in our AMG (Adaptive Multigrid) code (Suisalu & Saar

In contrast, in our AMG (Adaptive Multigrid) code (Suisalu & Saar 1995) the solution for local subgrids is obtained simultaneously with the global solution using the full multigrid method (Brandt 1977). According to the above classification AMG uses two-way grid interfaces between finer and coarser grids, as information passes in both directions during iterations. The reason why we have been left alone in this class is that here it is harder to get good convergence of the iterative solution process. We believe that two-way interfaces, once they have been built, are closer to the exact solution, and we shall use below our AMG-code for comparison with the AP^3M -code.

At first we encountered difficulties in building our models, as the natural boundary conditions for a multigrid code are the Dirichlet conditions, and our code was initially tuned for this case. In order to follow the evolution of spatially periodic P^3M models we had to modify our code for periodic boundary conditions.

If we use iterative methods to solve the Poisson equation on a grid, we discover that in the case of periodic boundaries the linearized system of algebraic equations that we have to solve becomes singular. Singular systems are more difficult to solve, and the problem becomes even harder if we consider interactions between the subgrids and the global grid. In the case of full two-way interfaces that we use, solutions on subgrids always induce changes in global solutions that violate global boundary conditions, and this usually requires additional iterations. In the periodic case the global solution is very sensitive to violations of the zero total mass condition that are generated by local subgrids, and convergence becomes very slow.

Sim.	L	N	ε	h _{min}		
P3M1*	32^{3}	32^{3}	0.2	1		
P3M2	32^{3}	32^{3}	1.0	1		
P3M3	32^{3}	32^{3}	2.0	1		
P3M4	32^{3}	64^{3}	0.2	1		
APM	32^{3}	32^{3}	0.2^{+}	1/8		
AMG1	32^{3}	32^{3}		1/16		
AMG2	32^{3}	64^{3}		1/32		
TREE	1	6440	0.2			
* Three different spectra						
[†] Short-range accelerations excluded						

Table 5.1: Simulation parameters

The remedy we chose was to use the Galerkin condition to modify the difference operators on coarser grids. Namely, we calculate the difference operator L^H on the coarse grid as

$$L^H = I_h^H L^h I_H^h, (5.1)$$

where L^h is the difference operator on the fine grid, I_h^H is the restriction operator from the fine grid to the coarse grid and I_H^h is the corresponding interpolation operator. This technique helps in the integration of singular systems, and it is described in detail by Hackbusch (1985). We found it essential for speeding up the convergence of the solution for the gravitational potential.

We chose to impose these conditions only when finding the solution for the global grid and did not modify the differential operator L on subgrids. In order to satisfy the boundary conditions themselves, we copied the appropriate boundary regions on global grids between iterations.

For P^3M simulations we used H. Couchman's Adaptive P^3M code AP^3M (Couchman 1991) that speeds up the normal P^3M by generating subgrids in regions of high particle density and finding a smooth solution for the potential there. This works to decrease the volume of pairwise force summation and considerably speeds up the algorithm. As concerns the adaptive smooth solution, the AP^3M -method belongs to the class of those with an one-way interface.

We have run and analyzed 6 P^3M simulations, 3 PM-type simulations and one tree-code simulation, their parameters are summarized in Table 5.1.
The first column labels the simulations, L is the base mesh size in cells (the physical size is $80h^{-1}$ Mpc for all simulations), N is the number of particles used, ε is the comoving softening parameter and h_{min} the minimal meshsize for adaptive models.

Couchman (1995) advises using softening radii that are constant in physical coordinates, which leads to increasing discreteness during simulations. While this could be appropriate to decribe the interaction of separate mass concentrations that may form during the simulation, it is certainly not the best description for dark matter. We used comoving softening to keep P^3M -simulations closer to smooth grid simulations; e.g., Gelb & Bertschinger (1994) have chosen the same approach.

Altogether we used three different values of the softening parameter $\varepsilon = 0.2, 1$ and 2 (our minimal softening is that normally used in P³M-simulations). The maximum number of refinement levels for AP³M was 4. The model we call APM is similar to the P3M1 with the only difference that we commented out in the source code the lines that updated velocities by accelerations from short-range forces – this is essentially a PM-model with adaptive mesh refinement, hidden inside the camp of AP³M-models.

Two other PM simulations labeled AMG1 and AMG2 were run using our Adaptive Multigrid code modified for periodic boundary conditions as described above. This code gives a spatial resolution for forces similar to that of P^3M codes without the need to consider pairwise forces. The last two codes differ by the number of points used and also by the number of subgrid levels allowed, 4 for AMG1 and 5 for AMG2.

The tree-code we used was the so-called 'Barnes' export' code with quadrupole corrections. While the computational volume for all other models was a periodic cube of size of $80h^{-1}$ Mpc, the volume for the tree-code was a sphere (with the same diameter). We used an opening angle $\theta = 0.8$ and physical coordinates with the timestep of 0.001 Gy.

We used the same initial conditions for all our models, trying to eliminate all possible sources of differences. The initial conditions were generated using the test power law spectrum with the spectral index n = -1 from the Couchman's Adaptive P³M distribution (see Couchman 1995 for a detailed description). For the P3M1-model we also generated two other realizations with the initial spectra being power laws with indices n = -2 and n = 0. When we compare different models from the Table 5.1, we use always those with the n = -1 spectrum.

As we simulated the simple $\Omega = 1$ cosmology, we could choose our starting time at will (we use the scalefactor *a* as our time variable). We started at a = 1 and followed the evolution until a = 9 when $\sigma_8 \approx 1$ for all



Figure 5.1: Particle distribution for the model P3M1 (P3M with a small softening parameter $\varepsilon = 0.2$) at the present epoch a = 9. The spectral index is n = -1 and the size of the cube is $80h^{-1}$ Mpc.



Figure 5.2: Particle distribution for the model AMG1 (AMG with 4 subgrid levels) at a = 9. The initial conditions and the cube size are the same as for the model P3M1 in Fig. 5.1.



Figure 5.3: The evolution of the initial density power spectrum P(k) (the curve marked a = 1) in different models. The spectra for the three models shown at the final moment a = 9 are labelled according to Table 5.1. The wavenumber k is given in comoving grid units.

models, thus we brought our models up to the present time. In order to study the growth of orbital deflections further, we followed the evolution of selected models for longer periods, up to a = 30.

We did not use the usual energy condition to check our time steps. Instead of this we use in our AMG code the Courant condition:

$$v_{max}\Delta a < 0.2h_{min},\tag{5.2}$$

(we change the time step when necessary, using an asymmetric leapfrog integration). As the AP³M-code uses a constant timestep, we first ran our AMG1-model, found the minimum timestep used ($\Delta a = 0.0625$) and used it for all simulations (we even ran AMG1 once more). This quarantees the use of the same algorithm for integration in time and eliminates one possible source of difference between models. The value of Δa we chose corresponds to $\Delta p = 0.01$ for the time variable p = (3/2)a used in AP³M for $\Omega = 1$. This time step is much smaller than usual, but it is necessary to accurately follow particle trajectories.

The typical density distribution for our models is shown in Figs. 5.1 and 5.2. The first one shows the particle distribution for the model P3M1 at a = 9 and the second one a similar one for the model AMG1. The

density distribution in the former seems to be more developed and has more distinct substructure, while AMG has retained more of linear structure elements and is less clumpy. We may suspect that the difference is due to pairwise collisions but we cannot say this on the basis of comparing density distributions only. The overall impression of both models is rather similar, of course — they start from identical initial conditions.

The evolution of the spectrum for different models was also rather similar (see Fig. 5.3). The difference is in the growth of small-scale modes that is the highest for the P^3M -models with a small softening (P3M1), the lowest for the APM model (this is essentially a pure PM-model) and intermediate for the smooth but high-resolution AMG1 run. The difference between the last two models can be explained by different depths of adaptive subgrid levels used (3 for APM and 4 for AMG1) and by the fact that the effective smoothing in P^3M is somewhat higher than that in AMG (about 3.5 versus 2 cell sizes). This makes the resolution achieved by AMG1 about 4 times higher than that in APM.

5.3 Deflection angles

It is well known that during the linear stage of growth of density perturbations particle velocities retain their initial directions; the well-known Zeldovich approximation says

$$\mathbf{x} = \mathbf{q} + \mathbf{b}(\mathbf{t})\mathbf{v}(\mathbf{q}),\tag{5.3}$$

where \mathbf{x} is the comoving coordinate of a particle labeled by its initial coordinates \mathbf{q} and b(t) is the density growth rate from the linear theory, a function of time only. This shows clearly that while the velocity amplitude may change in time, its direction remains fixed. In fact, the components of the velocity direction are adiabatic invariants of motion in the initial stage, while particle energies change with time even without any interaction. This suggests that the change of the velocity direction is a better measure of gravitational interaction than the usually used energy diffusion.

Nonlinear effects — growth of structure and pairwise collisions — both contribute to the change of the direction of velocity, and if we define the deflection angle $d\phi$ for a particle by

$$\mathrm{d}\phi = |\mathbf{v} \cdot \mathbf{d}\mathbf{v}| / \mathbf{v}^2, \tag{5.4}$$

then the total angle ϕ accumulated during the run of the simulation reflects all gravitational collisions suffered by the particle. The quantity ϕ does not describe the real angle between the initial and final direction of the velocity of a particle, as it omits the other degree of freedom θ necessary to describe a direction in a 3-D space. However, in case of a small total deflection the two angles are connected by

$$\langle \sin^2 \Phi \rangle = 2/3[1 - \exp(-3S/2)]$$
 (5.5)

(Standish & Aksnes 1969), where the accumulated square deflection for a trajectory S is

$$S = \sum_{a} (\mathrm{d}\phi)^2 \tag{5.6}$$

(a is our time coordinate). The mean in (5.5) concerns all trajectories with the same $d\phi$ -sequence but with different θ . For small values of S it is equal to the mean square of the final deflection angle Φ , but for a long history of collisions $\langle \sin^2 \Phi \rangle$ will reach the value 2/3 that describes an isotropic distribution. However, the accumulated square deflection S does not saturate and continues to describe the total effect of gravitational interactions. In this respect it is also better than the often-used measure of orbital divergence that saturates easily for spatially limited systems.

In order to be able to include the effects large single deflections we computed the deflection angles in the simulations as

$$d\phi = \arccos(\mathbf{v}_t \cdot \mathbf{v}_{t+\delta t} / |\mathbf{v}_t| |\mathbf{v}_{t+\delta t}|), \qquad (5.7)$$

this did not add significantly to the cost of the simulations. We summed both the deflection angles and their squares for every trajectory during a simulation.

After this work was finished, we learned about a similar measure proposed recently by Bagla & Padmanabhan (1995) to describe nonlinearity in cosmological structure formation. They describe deviations from the linear stage by a measure

$$D_{gu} = (\mathbf{u} - \mathbf{g})^2 / \mathbf{u}^2 \tag{5.8}$$

(as u is the velocity with respect to the dimensionless time a, its dimension is the same as that of the acceleration g). Their measure is easier to calculate than ours, but it has to be modified for other cosmologies (the Zeldovich approximation gives zero for this expression only for $\Omega = 1$ universe), ours does not depend on the background cosmology. But we see clearly that there are two sources for orbital deflections — nonlinear evolution of particle orbits in the smooth background field described by (5.8)

and the pairwise (gravitational) collisions we are looking for. Of course, both these sources contribute to the energy diffusion, too.

While deflection angles reflect histories of individual particles, the simplest characteristic describing the change of all particle trajectories in a simulation is the mean of accumulated squares of deflection angles for all trajectories $\langle S \rangle$. If particle motions are quasi-linear, as in the Zeldovich approximation, particles follow their initial direction (only their velocity may change in time) and $\langle S \rangle = 0$. Growth of the deflection angles describes nonlinear interactions, either via the mean field or by pairwise gravitational collisions.



Figure 5.4: Growth of the mean accumulated square deflection $\rangle S \langle$ with dimensionless time *a* (the scale factor). The models are labeled according to Table 5.1; the highest growth is observed in case of the P³M-models with a normal smoothing parameter $\varepsilon = 0.2$.

In Fig. 5.4 we see the evolution of the deflection measure $\langle S \rangle$ in time for different models. First we see a striking difference between the P³M-models with different smoothing parameters; for the normally accepted smoothing parameter ($\varepsilon = 0.2$) the accumulation of deflection angles is very rapid compared to those for larger ε . Contrary to the common belief, the rate of growth of deflection angles does not depend much on the total number of particles N — compare the curves P3M1 and P3M4, the latter is for a model with 8 times more particles than the P3M1. Our multigrid models lie in the middle of the range, the model AMG1 practically coinciding with the P3M2. This is understandable, as $\varepsilon = 1$ corresponds to a cell-sized smoothing; the model P3M3 $\varepsilon = 2$ is evidently 'oversmoothed'.



Figure 5.5: Growth of the mean squared angular velocity deflections $\langle W \rangle$ with dimensionless time a. The models are labeled according to Table 5.1; the highest growth is observed in case of the P³M-models with a normal smoothing parameter $\varepsilon = 0.2$.

Surprisingly, the model AMG2 gives larger deflections than the AMG1. This can hardly be caused by the larger number of particles, a much more likely cause is that we have allowed an extra level of refinement in this model and follow particle trajectories better. An additional source of deflections could be the force errors that each refinement introduces near subgrid boundaries; as we have shown earlier (Suisalu and Saar 1995), these errors are usually small, less than one per cent, but in rare cases they may reach a few per cent. Similar errors are present in the AP³M-code, where the usual requirement is to limit them to 6 per cent. We stress once more that this value describes very rare errors. Anyway, such errors may get amplified in a square-weighted characteristic such as $\langle S \rangle$. Another surprise is a relatively low deflection measure obtained for our tree-code run.

As we mentioned above, the deflection may be caused both by gravitational collisions and by interactions with the mean gravitational field. It is well known than in case of uncorrelated deflections particles follow a random walk in the energy space (see, e.g., Huang et al. 1993). This would translate in our case to

$$\frac{\mathrm{d}S}{\mathrm{d}a} = n(\Delta\phi)^2 \tag{5.9}$$

that would give a $\langle S \rangle \sim t$ dependence (*n* here is the mean frequency of collisions and $(\Delta \phi)^2$ the characteristic value of a single squared deflection). This is close to the *a*-dependence seen in Fig. 5.4.

However, in our nonstationary simulations we have to consider also the possible role of the mean-field effects. We can roughly model strong mean-field deflections, supposing that all particles rotate in circular orbits with angular velocities ω_i . In this case the computed deflection measure would grow as

$$\langle S(a)\rangle = \frac{1}{N} \sum_{i}^{N} \sum_{a} (\omega_{i} \Delta a)^{2} = \frac{a \Delta a}{N} \sum_{i} \omega_{i}^{2}.$$
(5.10)

As we see, $\langle S \rangle$ caused by a strong mean-field interaction is also proportional to time *a*, as the expected effect of collisions was.

In order to differentiate between the signatures of mean-field deflections and those caused by pairwise collisions, we introduced a new ('velocity') deflection measure W for the growth of the squared deflections of the angular velocity of a particle:

$$W(a) = \int_{a_0}^{a} \left(\frac{\mathrm{d}\phi}{\mathrm{d}a} - \omega\right)^2 \mathrm{d}a, \qquad (5.11)$$

where ω is the time-averaged rate of change of the deflection angle ω for a particle (the average angular velocity for planar orbits) during the whole simulation (from a_0 to a):

$$\omega = 1/(a - a_0) \int_{a_0}^a \frac{\mathrm{d}\phi}{\mathrm{d}a} \mathrm{d}a \qquad (5.12)$$

The velocity deflection measure W is, of course, zero for linear motions without a change of direction, but also for the case of strong interactions, when particles are trapped in systems and rotate with constant angular velocities ω_i , $\phi_i = \omega_i a$. In order to describe all particles we use a mean value of this measure $\langle W \rangle$. The growth of this measure in time for our simulations is shown in Fig. 5.5.

The difference between the mean velocity deflection measure for various models (Fig. 5.5) is considerably smaller than it was for the mean squared deflections (Fig. 5.4). The P3M1-model leads the pack as before, with its many-particle version close behind, and the tree-code model has generated similar deflections to the high-resolution AMG1. All other models are relatively quiet.



Figure 5.6: Growth of the velocity deflection measure $\langle W \rangle$ in the model P3M1 for different initial spectra with exponents n = 0, n = -1 and n = -2. The dotted line shows a power law $\langle W \rangle \sim a$.

We studied the $\varepsilon = 0.2$ case in more detail, trying to understand better the source of deflections. We continued the run deeper into nonlinear times (Fig. 5.6). We can see that the growth, although rather rapid at the start of the simulation (this rise could be probably explained by non-self-consistent starting conditions), levels off to a power law with the exponent $\alpha \approx 1$. As we have largely eliminated the mean-field effects, we may hope that this exponent tells us that the observed growth of $\langle W \rangle$ is caused by two-body effects. In order to check if this exponent depends on the large-scale environment we repeated the simulations for the model P3M1 for two more power spectra with the exponents n = -2 and n = 0. As can be seen from Fig. 5.6, the deflections grow in a similar fashion, and the exponents are practically the same – the curves differ by a multiplicative factor only. Examination of density distributions confirms that structure is much stronger in the n = -2 case, the n = 0 spectrum giving rise to a large number of small clumps and a rather diffusive sea of particles in between. This will naturally lead to a larger collision rate for the former model.



Figure 5.7: Distribution of the velocity deflection measure W for all particles in the P³M-model P3M1 for different moments a. The signature of high-deflection gravitational collisions is clearly seen as the right maximum. Observe how the distribution that is dominated by small deflections at the start of the simulation shifts gradually over to relatively large deflections.

It is clear that different particles follow extremely different orbits, and in order to understand their evolution it is better to 'differentiate' the average quantitities shown in Figs. 5.5-5.6 and to study the distributions of the velocity deflection measure for our collection of trajectories.

Fig. 5.7 demonstrates the evolution of this distribution in time for the collisional model P3M1. The main feature of this distribution is the presence of two strong maxima at all times. We may suppose that the left

maximum at smaller deflections is describing mean-field effects and the right maximum — gravitational collisions. During the evolution the number of particles that participate in collisions grows steadily. We see also a gradual shift of the distributions towards larger deflections — the accumulated velocity deflections grow. The width of the right maximum that can be thought of as describing the number of strong collisions (about 3 per unit logarithmic interval) grows also.

Similar distributions for the multigrid model AMG1 are shown in Fig. 5.9. They are distinctly different from the P^3M model shown before, having only one small-deflection maximum. During evolution the distribution spreads and only the last distribution that corresponds to highly nonlinear stages of evolution of structure (more than two present lifetimes of the Universe into the future) shows presence of an appreciable high-deflection tail. This tail is caused by the growth of small-scale substructure by far beyond the present epoch.



Figure 5.8: Distribution of the velocity deflection measure W for the APM-model (without local forces) at different times. The distribution is initially smoother than for the multigrid models in Fig. 5.9, and the final highly nonlinear stage develops similar fluctuations.

Even smoother distributions can be found when running the APM model, where the local pairwise forces were ignored. The distributions



Figure 5.9: Distribution of the velocity deflection measure W for the multigrid model AMG1 for different moments. The deflection measure grows gradually, but small deflections dominate at all times.

(Fig. 5.8) show only the signature of mean-field forces and practically do not evolve at all. This shows, first, a total absence of gravitational collisions typical for its parent P^3M -model, but also less substructure than in the AMG1-model (the spatial resolution of the present model was about 4 times lower than that of the AMG1). An exception is the distribution for large times that shows features similar to the AMG1, with even slightly larger amplitudes.

The tree-code shows features in between of P3M1-model and the smooth models — the distribution of the velocity deflection measure W (Fig. 5.10) is rather wide, comparable to that of the model P3M1, but it has only one maximum at all times. As the transformation between the physical time coordinate t used here and the 'scale factor time' a used for other models is nonlinear, it is difficult to compare these distributions directly with the W-distributions for other models. Even the strong-field approximations (5.10) do not agree with each other, and the measure W here implies a non-constant mean angular velocity with a.

As we saw above, the overall growth of the deflection measure was



Figure 5.10: Distribution of the velocity deflection measure W for the tree-code simulation at different times. The distribution is rather wide, but has only one maximum at all times.



Figure 5.11: Distribution of the velocity deflection measure W at the final stage of simulations for P³M-models with different softening parameters. The role of collisions (the right maximum) decreases rapidly with a growing ε .

similar for our multigrid models and for the P³M-models with rather large softening parameters (Fig. 5.4). The comparison of the distributions of the velocity deflection measure W at the end of the simulations, a = 9 for the P³M-models with different softening is shown in Fig. 5.11. Only the standard model P3M1 ($\varepsilon = 0.2$) shows a strong collision signature, for the smooth model P3M2 ($\varepsilon = 1$) the right maximum is already very weak and the 'oversmoothed' P3M3 ($\varepsilon = 2$) shows only mean-field deflections. It is even smoother than the APM-model, where the local pairwise interactions were ignored. We see also that the models with a large softening develop much smaller accumulated deflections.

The deflection characteristics we have studied so far have all been accumulated from the start of the simulation. As the deflection angle is positively defined, the change of its mean value, describing smooth-field effects, will contribute to some extent to the velocity deflection parameter W. We show a typical distribution of ω in Fig. 5.12 for the model AMG1. Its time dependence is rather slow, but ω tends to grow, and this may influence the accumulated velocity deflections.



Figure 5.12: Distribution of the mean angular velocity ω for different moments (the model AMG1). The initially concentrated distribution spreads in time both due to collisions and mean-field effects.

In order to eliminate this effect, we performed another 'differentiation' step, separating the overall evolution into a number of time intervals $a \in [a_i, a_{i+1}]$ and calculating the rate of growth of the velocity deflection measure (deflection rate) U using

$$U = W(a_i, a_{i+1}) / (a_{i+1} - a_i), \tag{5.13}$$

where $W(a_i, a_{i+1})$ is the same expression as in (5.11, 5.12) but we have changed the integration limits from (a_0, a) to (a_i, a_{i+1}) . It is important to keep in mind that this operation does not substract distributions at different times, we differentiate along the accumulated angular velocity deflections.

In Fig. 5.13 we see again the results for the P3M1-simulation. The picture is essentially the same as in Figure 5.7. Only the distributions for different times are more similar, and the roles of small deflections for a subinterval (mean-field effects) and those of large deflections are more clearly separated. The small-scale peaks do not move, indicating that the mean-field effects stay the same during the evolution. We built a similar graph for the model P3M4 that differs from the present model only due



Figure 5.13: Distributions of the deflection rate U for the P³M-model P3M1 for different time intervals. The left maximum describes the mean-field effects while the right maximum describing collisions grows steadily.

to a larger number of particles. As suggested by the similar behaviour of the deflection measure S (see Fig. 5.4) the distributions are practically the same.

The distributions of the deflection rate in the adaptive multigrid code are shown in Fig. 5.14. The figure reveals noticable differences between the U-distribution for the first and successive time intervals. A probable reason for this is a rather non-self-consistent initial state that gives rise to initial transients (such transients were observed also by Hernquist & Barnes, 1990, in their analysis of tree-code models). There might be several reasons for this happening, either the presence of softening in the force law as supposed by Hernquist & Barnes, or the fact that Couchman uses initial velocities found directly from the Zeldovich potential, while a 'quiet start' prescription (Efstathiou *et al.* 1985) advises finding them on the basis of the generated density field. Models evolve rapidly away from this stage, but they acquire in the process a high-deflection tail of the distribution of the deflection measures. The later evolution is much quieter, with most of the deflections coming from small-amplitude mean-field accelerations. At yet



Figure 5.14: Distributions of the deflection rate U for the multigrid model AMG1. After the initial fast evolution towards a quasiequilibrium growth, most particles keep moving smoothly and only a small percentage of them suffers deflections that place them in the high-deflection tail of the distribution.

later times yet when higher resolution grids are used we see also a growth of the high-deflection tail. This could be partly a mean-field effect and could be partly caused by force errors. This tail is, however, much lower than that for the P3M1-model and there is no sign of any maximum. This figure also shows that the strong differences between the *W*-distribution for nonlinear stages (see Fig. 5.9) is due to a large difference between the moments when they were constructed, the deflection rate being practically the same at a = 9 and at a = 20.

It is instructive to compare Fig. 5.13 with Fig. 5.15, where the Udistribution from the APM simulation is shown. This shows the difference between trajectories of particles which undergo short-range accelerations and which do not. The APM distribution is in fact very close to that for AMG, but it almost does not have the long high-deflection tail. There are at least two reasons for this — firstly, the adaptive grids in the APM did not reach as deep as they did in the AMG-models, and secondly, the subgrid force calculation procedure used in the AP³M-approach might give



Figure 5.15: Distributions of the deflection rate U for the APM-model. Here one observes only the initial fast relaxation, but there are practically no collision events.

cleaner forces.

Extra gravitational collisions inherent to a N-body code can directly influence the conclusions that we make comparing our models to observations. As they generate additional velocity changes, their presence is reflected most clearly in the velocity distributions. These can be compared easily with observations and they influence the properties of the gravitationally bound systems that are born during the simulations. As an example, we analyzed the distributions of relative velocities for particle pairs for different codes.

The relative velocity vector between a pair of particles can be decomposed into the line-of-sight ('radial') component and into the component perpendicular to this direction ('tangential') (see Gelb 1992). The radial component v_{\parallel} can be defined as

$$v_{||} = \frac{(\mathbf{v_1} - \mathbf{v_2}) \cdot (\mathbf{x_1} - \mathbf{x_2})}{|\mathbf{x_1} - \mathbf{x_2}|}$$
(5.14)

and the perpendicular velocity component v_{\perp} as



Figure 5.16: Dependence of the pairwise longitudinal ("radial") velocity dispersion $\sigma(v_{\parallel})$ (panel a) and the transversal velocity dispersion ("rotation velocities") $\sigma(v_{\perp})$ on the width of particle pairs r for different models. We see that the dispersion obtained from the P³M-models is much larger than that obtained from the smooth models, even at relatively large distances.

$$v_{\perp} = ((\mathbf{v_1} - \mathbf{v_2})^2 - \mathbf{v}_{\parallel}^2)^{1/2}.$$
 (5.15)

The dispersions of these velocities are shown in Fig. 5.16 for the final moment a = 9, corresponding roughly to the present epoch, for three different models, P3M1, AMG1 and APM. This figure shows that the P³Mcode gives velocity dispersions that are about 50% larger than we get using smooth-field codes to model the same patch of the Universe. The results we have seen above let us suspect that this difference may be mainly due to two-body effects in the P³M-code. And as we already mentioned, this could affect the conclusions one makes about the rotation velocities and masses of the systems that form and about the ease they form with.

5.4 Conclusions

We have compared a range of P^3M -models with different softening parameters and spectra and smooth-density models of comparable spatial resolution (APM, multigrid). We have seen that smooth-field PM-codes are considerably less collisional than the P^3M -codes. We have found that even when choosing comoving softening parameters instead of physical ones there is a considerable amount of gravitational collisions in standard P^3M -models. If their influence is crucial for the problem the simulation is run for (e.g. the study of velocity dispersions or of the formation of bound systems), we would recommend the use of comoving softening parameters $\varepsilon \ge 1.0$.

We have also proposed a new approach to the study of gravitational collisions in nonstationary systems that are common in cosmological simulations. We use measures based on the accumulated deflection angles of particle orbits and on accumulated angular velocity deflections. These measures are similar to the commonly used energy diffusion and orbit divergence measures, but they do not saturate during evolution.

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Suuremastaabilise struktuuri elementide evolutsiooni modelleerimine adaptiivse mitmevõre meetodiga

Kokkuvõte.

Käesolev dissertatsioon on kogumik autori avaldatud artiklitest, mis annab ülevaate adaptiivse mitmevõre meetodi väljatöötamisest ja rakendamisest kosmoloogilises modelleerimises.

Esimene peatükk (artikkel I publitseeritud artiklite nimestikust) kirjeldab suuremastaabilise struktuuri evolutsiooni analüüsi tulemusi, mis on saadud erilist tüüpi varjatud aine jaoks. Vastav artikkel on kirjutatud juba mõni aeg tagasi ning ta oli üks esimesi, kus toodi sisse uut tüüpi varjatud aine — nn. külm varjatud aine, mis on muutunud standardseks Universumi varjatud aine mudeliks tänapäeval. Seal rakendatakse samu numbriliste mudelite ja vaatluste võrdlusmeetodeid, mis on kasutusel praegugi ning puudutatakse teoreetilisi probleeme, mis on aktuaalsed ka nüüdsel ajal. Ta on samuti esimene artikkel, kus klasteranalüüsi kasutatakse numbriliste mudelite analüüsiks. Kokkuvõttes annab see peatükk küllalt põhjaliku ülevaate Universumi suuremastaabilise struktuuri numbrilise mudelleerimise probleemidest, mis valdavalt on ikka veel lahendamata.

Teine peatükk (artikkel III) ehitab baasi galaktikate superparvede tekkimise teooriale. Uuenduseks selles on varjatud aines moodustuvate struktuuride tüü-pilisele geomeetriale vastavate algkiiruste väljade otsene tuletamine Lagrange'i singulaarsuste teooriast. Selles peatükis on antud teooria küllalt põhjalik ülevaade ja toodud standardsete algkiiruste väljade, mis peaksid eksisteerima üldisel aine liikumisel omaenda gravitatsiooni mõjul, tuletus. Need algkiiruste väljad on baasiks edasisel galaktikate superparvede tekke mudelleerimisel, kasutades adaptiivse multivõre meetodit.

Kolmandas peatükis (artikkel II) tutvustatakse isegraviteeruvate struktuuride evolutsiooni mudelleerimist mitmevõre meetodiga. Siin võrreldakse kahte võistlevat meetodit Poissoni võrrandi lahendamiseks: üks, kus kasutatakse Kiiret Fourier Teisendust, ning mis on enim kasutatav praegusel ajal, ja teine on mitmevõre variant. Tulemused näitavad, et viimane meetod on on küllaltki võrreldav Kiirel Fourier Teisendusel baseeruva meetodiga, kui silmas pidada arvutuslikke parameetreid (nagu mälu vajadus, kiirus jne.) ja füüsikalisest seisukohast paistab mitmevõre meetod parem olema mudelleerimaks ühemõõtmelist sfäärilist kollapsit (näide on valitud kui üks vähestest gravitatsioonilises dünaamikas tuntud täpsetest lahenditest). Neljandas peatükis (artikkel V) tutvustatakse täielikku kolme-mõõtmelist adaptiivset mitmevõre koodi, mis on kirjutatud autori poolt (see on ka dissertatsiooni põhitulemus) ja kirjeldatakse tema testimist kosmoloogilistel rakendustel. Rakendusena on kasutatud pankoogi-laadse struktuuri teket (kui lihtsaim singulaarsus peaks see kirjeldama kõige rohkem levinud struktuurielemendi geomeetriat), kasutades algkiiruste välja, mis on tuletatud Peatükis 2. See peatükk näitab adaptiivse mitmevõre meetodi suurt ruumilist lahutusvõimet. Me oleme saavutanud siin esimest korda (lineaarse) lahutuse L/1024, kus L on arvutuspiirkonna (kuubi) mõõde, kasutades ainult Sun'i tööjaama. Sellist ruumilist lahutust pole veel saavutatud isegi tänapäeva superarvutitel; meie eelis on selles, et adaptiivne mitmevõre meetod kasutab suuremat lahutust seal, kus see on vajalik, mitte aga igal pool üle arvutuspiirkonna, nagu on tarvis teha kui kasutada Kiiret Fourier Teisendust.

Viiendas peatükis (artikkel VI) võrreldakse kõiki enim kasutatavaid kosmoloogilise struktuuri tekke mudelleerimise N-keha-meetodeid (nagu PM, $P^{3}M$, adaptiivne $P^{3}M$, puu-kood ja adaptiivne mitmevõre kood), uurides nende gravitatsioonilist põrkelisust, mis on põhjustatud aine pideva jaotuse esitamisest diskreetsete osakeste abil. Selleks kasutatakse uut kahe-keha relaksatsiooni mõõtu, mis põhineb osakeste kumulatiivsetel orbitaalsetel suunamuutustel. Analüüs näitab, et P³M tüüpi koodis on gravitatsiooniliste põrgete osa küllalt suur, mis on ootamatu tulemus ning sunnib suhtuma seda tüüpi mudelitesse kriitiliselt. Adaptiivne multivõre meetod on selles suhtes palju parem, siiski vajab jõu leidmine alam(suurema lahutusega)võre äärtel edasist tööd; jõu fluktuatsioonid seal võivad põhjustada samuti suurendatud orbitaalseid suunamuutusi, kuid siiski palju väiksemas ulatuses kui osakeste gravitatsioonilised põrked P³M meetodis. See näitab samuti, et mitmevõre meetodiga on kindlasti parem mudelleerida struktuuri teket (varjatud aines) kui teiste praegu kasutatavate populaarsete meetoditega.

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