

Victor G. Ganzha
Ernst W. Mayr
Evgenii V. Vorozhtsov (Eds.)

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Computer Algebra in Scientific Computing

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Proceedings

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Preface

This volume contains revised versions of the papers submitted to the workshop by the participants and accepted by the program committee after a thorough reviewing process. The collection of papers included in the proceedings covers not only various expanding applications of computer algebra to scientific computing but also the computer algebra systems themselves and the CA algorithms.

The eight earlier CASC conferences, CASC 1998, CASC 1999, CASC 2000, CASC 2001, CASC 2002, CASC 2003, CASC 2004, and CASC 2005 were held, respectively, in St. Petersburg, Russia, in Munich, Germany, in Samarkand, Uzbekistan, in Konstanz, Germany, in Crimea, Ukraine, in Passau, Germany, in St. Petersburg, Russia, and in Kalamata, Greece, and they proved to be successful.

It was E.A. Grebenikow (Computing Center of the Russian Academy of Sciences, Moscow) who drew our attention to the group of mathematicians and computer scientists at the Academy of Sciences of Moldova conducting research in the field of computer algebra. We were impressed that this group not only is concerned with applications of CA methods to problems of scientific computing but also carries out research on the fundamental principles underlying the current computer algebra systems themselves, see also their papers in the present proceedings volume. It was therefore decided to organize the 9th workshop on Computer Algebra in Scientific Computing, CASC 2006, in Chişinău, the capital of Moldova. We hope that this will foster new and closer interactions between the Moldova CA group and other research groups working in the field of computer algebra.

The papers collected in the present volume are devoted both to the topics that have already become traditional for the CASC workshops, and to several new topics. Among the traditional topics, there are the studies in Gröbner bases, polynomial algebra, homological algebra, quantifier elimination, the applications of computer algebra systems in the field of the solution of differential equations, celestial mechanics, Newton polyhedra, mathematical physics, nuclear physics, and fluid dynamics.

Two papers present the results in a new topic, which was addressed for the first time during the CASC 2005 workshop: the application of computer algebra techniques in the field of nanosciences and nanotechnology. Another novel theme is the application of CA methods to cellular automata with symmetrical local rules.

In addition to the accepted submissions, this volume also includes two invited papers. The paper by T. Sturm (University of Passau) addresses various aspects of the computer-algebra-based computer logic system REDLOG, which focuses on real quantifier elimination algorithms. An immense potential of quantifier elimination techniques for the integers is pointed out. Another new REDLOG domain is queues over arbitrary basic domains. Both have promising applications in practical computer science, viz. automatic loop parallelization and software security.

The invited talk by S.M. Watt (University of Western Ontario) is devoted to algorithms for symbolic polynomials where the exponents are not known in advance, such as $x^{2n} - 1$. The case is considered where multivariate polynomials can have exponents which are themselves integer-valued multivariate polynomials, and algorithms are presented to compute their GCD and factorization. Additionally, the case of symbolic exponents on rational coefficients (e.g., $4^{n^2+n} - 81$) is treated, and it is shown how to avoid integer factorization.

Our particular thanks are due to the members of the CASC 2006 local organizing committee at the Technical University of Moldova: V. Dorogan (Chair), M. Izman, and V. Dragan, who have ably handled local arrangements in Chişinău. We are grateful to W. Meixner for his technical help in the preparation of the camera ready manuscript for this volume.

July 2006

V.G. Ganzha
E.W. Mayr
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V. Álvarez, J.A. Armario, M.D. Frau, and P. Real

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Abstract. Let A be a commutative ring, A an augmented differential graded algebra over A (briefly, DGA-algebra) and X be a relatively free resolution of A over A . The standard bar resolution of A over A , denoted by $B(A)$, provides an example of a resolution of this kind. The comparison theorem gives inductive formulae $f: B(A) \rightarrow X$ and $g: X \rightarrow B(A)$ termed comparison maps. In case that $fg = 1_X$ and A is connected, we show that X is endowed a A_∞ -tensor product structure. In case that A is in addition commutative then (X, μ_X) is shown to be a commutative DGA-algebra with the product $\mu_X = f * (g \otimes g)$ ($*$ is the shuffle product in $B(A)$). Furthermore, f and g are algebra maps. We give an example in order to illustrate the main results of this paper.

1 Introduction

Calculations in homological algebra are commonly expressed in terms of resolutions. It is not unusual that these resolutions are embedded in the bar construction (or some other standard resolution) in a special way. When this occurs, they are said to *split off* of the standard resolution (see [14]).

A classic example is the Koszul resolution $K = A \otimes E_A[u_1, \dots, u_n]$ related to the ideal $I = (x_1, \dots, x_n)$ in the polynomial ring $A = A[x_1, \dots, x_n]$; as A is an augmented algebra over A , the *bar resolution* $B(A)$ for A over A [5, 16] can be constructed. K is also a resolution of A over A and by the comparison theorem [16], there is a chain homotopy equivalence $B(A) \leftarrow K$. In this case, an explicit contraction (special homotopy equivalence) $B(A) \Rightarrow K$ exists [17]. This contraction makes that the Koszul resolution splits off of the bar resolution. Using this contraction and some homological perturbation tools, perturbations of this resolution can be computed and the perturbed resolutions can be used to make complete effective calculations where previously only partial or indirect results were obtainable. This idea has been exploited in a series of papers by Lambe [12, 13, 14] and provides an algorithm for computing resolutions *which split off of the bar construction*. This algorithm has been extended to a more

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general context in [11]. We point out that the notion of contraction is essential in order to find effective algorithms in homological algebra using the set of techniques provided by homological perturbation theory, since the input data of our algorithm have to be codified in this form.

The well-known comparison theorem in homological algebra states that any two projective resolutions are chain homotopy equivalent. For relatively free resolutions $Y = A \otimes \bar{Y}$ and $X = A \otimes \bar{X}$ of A over A with explicit contracting homotopies, there are recursive procedures for obtaining explicit equivalences $f: Y \rightarrow X$ and $g: X \rightarrow Y$ where the explicit contracting homotopies play a principal rule. In addition, there are inductive procedures for obtaining explicit chain homotopies of fg and the identity and with gf and the identity. Generally, the maps defined in this way do not form a contraction. Here, assuming that $Y = B(A)$, we give a necessary and sufficient condition for determining when these maps form a contraction, which seems to be new.

In the special case that A is connected, Y is the bar resolution of A over A , and the above maps form a contraction from $B(A)$ to X (i.e., X is a resolution which splits off of the bar resolution), we define a degree minus one map $\tau: \bar{X} \rightarrow A$ which is an A_∞ -twisting cochain, so that $(X, \tau, \{\Delta_i\}_{i \geq 0})$ becomes an A_∞ -twisted tensor product where $\{\Delta_i\}_{i \geq 0}$ is the A_∞ -coalgebra structure of \bar{X} transferred from $\bar{B}(A)$ by means of ‘tensor trick’ [8] (see Algorithm 1). This provides an elegant codification of the differential of the complex X in terms of the A_∞ -twisting cochain and the A_∞ -coalgebra structure of \bar{X} . Furthermore, assuming in addition that A is commutative (but not necessarily connected) and that the contracting homotopy of X is a quasi algebra homotopy (see [19]), we prove that the morphism $\mu_X = f * (g \otimes g)$ ($*$ is the shuffle product in $B(A)$) endows X a commutative algebra structure, for which f and g are algebra maps (see Theorem 7) and give a method for computing new resolutions taking advantage of this algebra structure (see Algorithm 2). In the example given in this paper, we compute a resolution \tilde{X} of \mathbf{Z}_p over $\Gamma(w, 2n)$ using an initial resolution which splits off of the standard resolution, $B(A) \Rightarrow X$, and perturbing this contraction. The contraction $B(A) \Rightarrow X$ has been computed by means of the comparison theorem. We prove that X is a DGA-algebra as well as \tilde{X} . A computational advantage is deduced from this fact, since it is only necessary to compute the perturbed differential on the generators of \tilde{X} as an algebra, better than on the whole set of generators as a module. This type of computational advantage is our main motivation for studying the algebra structures underlying the resolutions.

We organize the paper as follows. In section 2 we give the necessary definitions and notations for defining the comparison maps when Y is the bar resolution and X is a contractile relatively free resolution. We also give a necessary and sufficient condition for guaranteeing that a contraction arises. Section 3 is devoted to study the A_∞ -structure inherent in X , when X is a relatively free resolution over a connected DGA-algebra A . In section 4 we analyse the multiplicative behaviour of the comparison maps, assuming that A is a commutative DGA-algebra and that the contracting homotopy of X is a quasi algebra homotopy. Finally, we give an example in order to illustrate the main results of the paper.

2 The Canonical Comparison Contraction – A Necessary and Sufficient Condition

We will quickly review some basic notions of Homological Algebra. More details can be found in [16]. Let A be a commutative ring with $1 \neq 0$, and A an augmented differential graded algebra over A , briefly termed DGA-algebra. The differential, product, augmentation and coaugmentation of A will be denoted respectively by d_A , μ_A , ϵ_A , and η_A . Nevertheless, sometimes, we will write them simply by d , μ , ϵ , and η when no confusion can arise. In what follows, the Koszul sign conventions will be used. A morphism $\rho : A_* \rightarrow A_{*-1}$ is called *derivation* if it is compatible with the algebra structures on A . The degree of an element $a \in A$ is denoted by $|a|$. Let us recall that if B is also a DGA-algebra, then $A \otimes B$ is canonically endowed an algebra structure by means of the morphism $\mu_{A \otimes B} = (\mu_A \otimes \mu_B)(1_A \otimes T \otimes 1_B)$, where $T(b \otimes a) = (-1)^{|b||a|}a \otimes b$. If the DG-algebra A is connected, that is $A_0 = A$ and $d_1 : A_1 \rightarrow A_0$ is zero, then there is a canonical augmentation $\epsilon_A = 1_A : A_0 \rightarrow A$.

Let n be a positive integer. The exterior algebra with one generator u in degree $2n - 1$, the polynomial algebra with one generator v in degree $2n$, and the divided power algebra with one “generator” w in degree $2n$ are denoted by $E(u, 2n - 1)$, $P(v, 2n)$, and $\Gamma(w, 2n)$, respectively.

We need here the *reduced bar construction* $\bar{B}(A)$ of a DGA-algebra A (see [16]). Recall that it is defined as the connected DGA-coalgebra, $\bar{B}(A) = T^c(S(\bar{A}))$, where $T^c(\)$ is the tensor coalgebra, $S(\)$ is the suspension functor, and $\bar{A} = \text{Ker } \epsilon_A$ is the augmentation ideal of A . The element of $\bar{B}_0(A)$ corresponding to the identity element of A is denoted by $[\]$ and the element $S\bar{a}_1 \otimes \cdots \otimes S\bar{a}_n$ of $\bar{B}(A)$ is denoted by $[a_1 | \cdots | a_n]$. The tensor and simplicial degrees of the element $[a_1 | \cdots | a_n]$ are $||[a_1 | \cdots | a_n]||_t = \sum |a_i|$ and $||[a_1 | \cdots | a_n]||_s = n$, respectively; its total degree is the sum of its tensor and simplicial degree. The tensor and simplicial differential are defined by:

$$d_t([a_1 | \cdots | a_n]) = - \sum_i (-1)^{e_i-1} [a_1 | \cdots | d_A(a_i) | \cdots | a_n],$$

and

$$d_s([a_1 | \cdots | a_n]) = \sum_i (-1)^{e_i} [a_1 | \cdots | \mu_A(a_i \otimes a_{i+1}) | \cdots | a_n]$$

where

$$e_i = i + |a_1| + \cdots + |a_i|.$$

If the product of A is commutative, a product $*$ (called shuffle product) can be defined on $\bar{B}(A)$. In this way, the reduced bar construction has a commutative Hopf algebra structure.

We will use here the structure of *twisted tensor product*. Let A be a DG-algebra and C a DG-coalgebra. It is well known that $\tau : C_* \rightarrow A_{*-1}$ is a *twisting cochain* if and only if $d^\tau = d_A \otimes 1 + 1 \otimes d_C + \tau \cap$ is a differential on $A \times C$ (see [4]), where the morphism $\tau \cap$ is defined by:

$$\tau \cap = (\mu_A \otimes 1)(1 \otimes \tau \otimes 1)(1 \otimes \Delta_C). \quad (1)$$

The DG-module $(A \otimes C, d^\tau)$ is called *the twisted tensor product (or TTP) of A and C along τ* . We will also use the notation of $A \otimes_\tau C$ for such DG-module.

A *relatively free resolution of A over A* is a pair (X, ϵ) where X is a graded differential A -module of the form $X = A \otimes_A \bar{X}$ with \bar{X} a DG- A -module and $\epsilon: X \rightarrow A$ a morphism of graded differential A -modules which is a weak equivalence, thereby, the homology of X is zero except in degree 0 where it is A . We will call the complex $(\bar{X}, d_{\bar{X}})$ the reduced complex, and it is always obtained in the form $(\bar{X}, d_{\bar{X}}) = (A \otimes_A X, 1_A \otimes_A d_X)$, by means of the the classical ‘neglect’ functor on the category of all A -modules to the category of all A -modules. It is standard terminology to call the elements of \bar{X} reduced elements. Given a morphism $\psi: X \rightarrow Y$ the notation $\psi|_{\bar{X}}(\bar{x})$ means $\psi(1 \otimes \bar{x})$ where 1 is the unit in A and $\bar{x} \in \bar{X}$. We follow these conventions throughout the paper.

A resolution $\epsilon: (X, d) \rightarrow A$ is called *contractile* if there exists a ‘contracting homotopy’, i.e., a family of A -module morphisms, $h_{-1}: A \rightarrow X_0$, $h_n: X_n \rightarrow X_{n+1}$, such that $1 = d_{n+1}h_n + h_{n-1}d_n$, $\forall n \geq 0$, where $d_0 = \epsilon$ and $h_{-1} = \eta$. Besides, it may always be assumed to hold that $h^2 = 0$ (see [3]).

Throughout this paper, (X, h, d) will denote a contractile relatively free resolution (X, d) with contracting homotopy h .

An important example of relatively free and contractile resolution of A over A is the *bar resolution* $(B(A), s, d)$ (or $B(A)$) [16, 13]. More specifically, $B(A)$ is the *twisted tensor product* $A \otimes_\theta \bar{B}(A)$, where the twisting cochain θ is given by

$$\theta([a_1 | \cdots | a_n]) = \begin{cases} a_1 & n = 1 \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

where the weak equivalence $\epsilon_{B(A)}: B(A) \rightarrow A$ is the canonical augmentation of $B(A)$ (in fact, it is a homotopy equivalence) and the contracting homotopy s is given by

$$s: B(A) \rightarrow B(A) \quad \text{where} \quad s(a \otimes [a_1 | \cdots | a_n]) = [a | a_1 | \cdots | a_n].$$

From now on, we will use s for denoting the above homotopy.

A *contraction* (see [6], [9]) is a data set $c: \{N, M, f, g, \phi\}$ where $f: N \rightarrow M$ and $g: M \rightarrow N$ are morphisms of DG-modules (called, respectively, *projection* and *inclusion*) and $\phi: N \rightarrow N$ is a morphism of graded modules of degree +1 (called *homotopy operator*). These data are required to satisfy the rules: **(c1)** $fg = 1_M$, **(c2)** $\phi d_N + d_N \phi + gf = 1_N$ **(c3)** $\phi \phi = 0$, **(c4)** $\phi g = 0$ and **(c5)** $f \phi = 0$. These three last are called side conditions [15]. In fact, these may always be assumed to hold, since the homotopy ϕ can be altered to satisfy these conditions [7, 14]. We will also denote a contraction c by $(f, g, \phi): N \Rightarrow M$.

For instance, the bar resolution $B(A)$ of a DG-algebra A gives the following contraction:

$$C_{B(A)}: \{B(A), A, \epsilon_{B(A)}, \eta_{B(A)}, s\} \quad (3)$$

where $\eta_{B(A)}: A \rightarrow B(A)$ is the canonical coaugmentation of $B(A)$.