

# About parallelizing the search for 3-dim. scalar discrete integrable equations

T. Wolf

Brock University, Ontario, Canada  
twolf@brocku.ca

W. Neun

Konrad Zuse Institut, Freie Universität Berlin, Germany  
neun@zib.de

Sergey P. Tsarev

Technical University Berlin, Germany  
sptsarev@mail.ru

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# Outline

## Discrete Differential Geometry

3d Faces that are 4d Consistent

Difficulties

Simplifications

Cubical Symmetry

Probing

Filling Holes by Digging new Ones

Solutions

Parallelization of the Computation

Guidance Principles

Overall Structure

Case Splitting

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Safety

To Do

## 2d Faces that are 3d Consistent

The object of interest is an affine linear relation

$$0 = Q := q_0 + q_1 f_{00} + q_2 f_{01} + \dots + q_{15} f_{00} f_{01} f_{10} f_{11}$$

between 4 scalar values  $f_{00}, f_{01}, f_{10}, f_{11}$  attached to the 4 corners of a square. This is called a ‘face relation’. It allows to compute any one of the 4 values  $f_{ij}$  from the 3 others.

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Of interest are such relations, i.e. values of coefficients  $q_0, \dots, q_{15}$ , which are *3d consistent* in the following sense.

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- ▶ Given are the 4 independent values  $f_{000}, f_{001}, f_{010}, f_{100}$ .
- ▶ Use 3 face relations to compute  $f_{011}, f_{101}, f_{110}$ .
- ▶ Use the remaining 3 face relations to compute  $f_{111}$  three times.
- ▶ The three expressions for  $f_{111}$  must coincide for arbitrary values of the independent  $f_{000}, f_{001}, f_{010}, f_{100}$ .
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This type of computation has been done before by Adler, Bobenko and Suris. Our aim is to compute 3d faces that are 4d consistent. For more details see

Tsarev, S.P. and Wolf, T.: Classification of 3-dimensional integrable scalar discrete equations, preprint, 19 pages, arXiv:0706.2464

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# The Setup

- ▶ **affine linearity of  $Q$ :**

A 3d cube has  $2^3 = 8$  corner values  $f_{000}, f_{001}, \dots, f_{111}$ ,

$$\rightarrow Q = q_0 + q_1 f_{000} + q_2 f_{001} + \dots + q_{255} f_{000} f_{001} \dots f_{111}$$

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► **4d consistency:**

- Use 4 face relations to compute  $f_{0111}, f_{1011}, f_{1101}, f_{1110}$  in terms of the 11 independent  $f_{0000}, f_{0001}, f_{0010}, \dots, f_{1010}, f_{1100}$ .
- Compute  $f_{1111}$  4 times from the remaining 4 face relations, require the equality of the 4  $f_{1111}$ , giving 3 relations to be fulfilled identically in the 11 independent  $f$ 's.
- Splitting wrt. the 11 independent  $f$ 's gives polynomial conditions for the unknowns  $q_\alpha$ .

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# Size of Conditions

dimension of face	$n$	2	3	4
# of $f$ -variables in face formula	$2^n$	4	8	16
# of terms in face formula (= # of undetermined coefficients $q_{\mathcal{D}}$ in $Q_n$ )	$2^{2^n}$	16	256	65536
# of all $f$ -variables in $(n+1)$ -dim. hypercube	$2^{n+1}$	8	16	32
# of indep. $f$ -variables in $(n+1)$ -dim. hypercube	$2^{n+1} - n - 2$	4	11	26
# of $n$ -dim. faces in $(n+1)$ -dim. hypercube	$2(n+1)$	6	8	10
# of consistency conditions	$n$	2	3	4
upper bound on the # of terms of each condition	$2^{\{2^{n+1}(n+1)-2n-1\}}$	$5.2 \times 10^5$	$1.4 \times 10^{17}$	$2.8 \times 10^{45}$
total degree of the $q_{\mathcal{D}}$ in each condition	$2n+2$	6	8	10
upper bound estimate of the # of equations resulting from splitting each condition	$2n(2n+2)^{(2^{n+1}-n-3)}$	864	$6.4 \times 10^9$	$8.0 \times 10^{25}$
estimated average # of terms in each equation	$\frac{2^{2^{n+1}(n+1)-2n-1}}{2n(2n+2)^{(2^{n+1}-n-3)}}$	606	$2.2 \times 10^7$	$3.5 \times 10^{19}$

Table: Size and number of consistency conditions

# Difficulties

1. Strictly speaking, in order to formulate even only the smallest subset of conditions one would have to formulate at least one consistency condition (by performing steps 1, 2 fully and 3 - 6 for at least two  $x_k = 1$  face relations before splitting) i.e. to generate an expression with  $2^{\{2^{n+1}(n+1)-2n-1\}}$  ( $= 1.7 \times 10^{17}$  for  $n = 3$ ) terms.

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2. If one found a way around this hurdle then the resulting equations are of high degree  $2n + 2$  with on average many terms.
3. Even if one were able to generate 100,000's of equations and thus find shorter ones which one could solve for some unknowns in terms of others, one would face the problem that many cases and sub-sub-cases have to be investigated due to the high degree of the equations.

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# Simplifications I

Cubical symmetry is characterized by 3  $\pm$  in

$$Q = \pm Q|_{x \leftrightarrow y} = \pm Q|_{y \leftrightarrow -y} = \pm Q|_{z \leftrightarrow -z}.$$

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For the hardest of these 3 symmetry types (+ + +) this leads to a reduction of the number of terms for each consistency condition from  $10^{17}$  to about  $10^{14}$  according to a study performed with the CA system FORM, although intermediate expressions are expected to have around  $10^{15}$  terms.

# Cubical Symmetry

The nonempty symmetry classes of formulas  $Q$  for face dimensions 2, 3, 4 are:

$n$	types of symmetry, number of parameters and terms	number of parameters in $SL_2$ -invariant subcases
2	(+-): 1 param.; 4 terms (-+): 3 param.; 10 terms (++): 6 param.; 16 terms	1 param.; 4 terms none 1 param.; 6 terms
3	(---): 1 param.; 24 terms (-++): 13 param.; 186 terms (+++): 22 param.; 256 terms	1 param.; 24 terms none 3 param.; 114 terms
4	(----): 94 param.; 29208 terms (+----): 77 param.; 26112 terms (-+++): 349 param.; 60666 terms (++++): 402 param.; $2^{16}$ terms	5 param.; 15480 terms none 3 param.; 15809 terms 18 param.; 96314 terms

**Table:** Symmetry classification of the face formulas w.r.t the complete symmetry group of the cube

# Simplifications II

## Probing

There are 11 independent (splitting) variables

$f_\alpha : f_{0000}, f_{0001}, \dots, f_{1100}$  (with at most two 1's in the index).

- ▶ replace some ( $:= z$ ) of the  $f_\alpha$  by zero,  
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  - (+) smaller expressions
  - (-) fewer split variables
- ▶ keep the remaining  $s := 11 - z - u$  variables  $f_\alpha$  symbolic.

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- ▶ solve the remaining equations in the solution process.

## Two Phases

1. Computing a solution by the above steps and generalizing to about  $z = 1, u = 0, s = 10$  (limited by memory), so close to the general case  $z = 0, u = 0, s = 11$ .

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(Later by performing a brute force test using the computer algebra system FORM solutions are checked again rigorously and independently but it needs a special order of substitutions to be able to complete the test.)

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- (-) accidental factorization of some face relations,
- (-) triangularization results in the need to generate many equations.

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- (+) Millions of equations that are identically satisfied modulo the preliminary solution do not get formulated.
- (+) Equations that get formulated are much shorter (involving only dozens or 100's of terms instead of 1000's or millions.
- (−) As the computation splits into cases and (sub−)<sup>10−15</sup>cases the generated conditions are only valid in the corresponding case and its sub-cases → very many files of generated equations (e.g. too many to do in unix: `rm *`).

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- (+) easy to do within CRACK with its flexible priority list. This needs just 2 more 'modules', one for generating a new file and one for reading from a file and it needs to find the right place for both modules within the priority list.
- (-) needs detailed programming if all should be done automatically for all sub-sub-cases.

# Accidental Factorization of Face Relations

We go back to the 2nd problem of ‘probing’.

For some face relation:  $0 = A_k(f_\alpha)f_{1..101..1} + B_k(f_\alpha)$   
it may be  $P_k := \text{GCD}(A_k, B_k) \neq 1$ .

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→ better split first  $P_k = 0 \rightarrow P_{kl} = 0$  and  $C_i = 0 \rightarrow C_{ij} = 0$  and consider the system  $0 = P_{kl} C_{ij} \forall l, i, j$ .

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Repeat this for each factor of each GCD from each substitution, also the substitution of  $f_{11..11}$ .

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- (+) CRACK keeps track of inequalities  
→ reduction of number of factors and thus equations,
- (+) Also, this package is well suited to handle case distinctions automatically.

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# Results

Case (+ + +) : 5 solutions

Case (- + +) : 3 solutions

Case (- - -) : 1 solution

# A Solution with (+ + +) Symmetry

$$\begin{aligned} Q = & q_{105} (f_{001} f_{010} f_{100} f_{111} + f_{000} f_{011} f_{101} f_{110}) + \\ & q_{107} (f_{001} f_{010} f_{100} f_{110} f_{111} + f_{001} f_{010} f_{100} f_{101} f_{111} + f_{001} f_{010} f_{011} f_{100} f_{111} + \\ & f_{000} f_{011} f_{101} f_{110} f_{111} + f_{000} f_{011} f_{100} f_{101} f_{110} + f_{000} f_{010} f_{011} f_{101} f_{110} + \\ & f_{000} f_{001} f_{011} f_{101} f_{110} + f_{000} f_{001} f_{010} f_{100} f_{111}) + \\ & \frac{q_{107}^2}{q_{105}} (f_{001} f_{010} f_{100} f_{101} f_{110} f_{111} + f_{001} f_{010} f_{011} f_{100} f_{110} f_{111} + \\ & f_{001} f_{010} f_{011} f_{100} f_{101} f_{111} + f_{000} f_{011} f_{100} f_{101} f_{110} f_{111} + \\ & f_{000} f_{010} f_{011} f_{101} f_{110} f_{111} + f_{000} f_{010} f_{011} f_{100} f_{101} f_{110} + \\ & f_{000} f_{001} f_{011} f_{101} f_{110} f_{111} + f_{000} f_{001} f_{011} f_{100} f_{101} f_{110} + \\ & f_{000} f_{001} f_{010} f_{100} f_{110} f_{111} + f_{000} f_{001} f_{010} f_{100} f_{101} f_{111} + \\ & f_{000} f_{001} f_{010} f_{011} f_{101} f_{110} + f_{000} f_{001} f_{010} f_{011} f_{100} f_{111}) + \\ & \frac{q_{107}^3}{q_{105}^2} (f_{001} f_{010} f_{011} f_{100} f_{101} f_{110} f_{111} + f_{000} f_{010} f_{011} f_{100} f_{101} f_{110} f_{111} + \\ & f_{000} f_{001} f_{011} f_{100} f_{101} f_{110} f_{111} + f_{000} f_{001} f_{010} f_{100} f_{101} f_{110} f_{111} + \\ & f_{000} f_{001} f_{010} f_{011} f_{101} f_{110} f_{111} + f_{000} f_{001} f_{010} f_{011} f_{100} f_{110} f_{111} + \\ & f_{000} f_{001} f_{010} f_{011} f_{100} f_{101} f_{111} + f_{000} f_{001} f_{010} f_{011} f_{100} f_{101} f_{110}) + \\ & 2 \frac{q_{107}^4}{q_{105}^3} (f_{000} f_{001} f_{010} f_{011} f_{100} f_{101} f_{110} f_{111}) \end{aligned}$$

# Trivialization

Möbius transformations keep  $0 = Q$  affine linear:

1.  $f_{ijk} \mapsto \frac{q_{105}}{q_{107}} f_{ijk}$  and  $Q \mapsto \frac{q_{107}^4}{q_{105}^5} Q$  (this eliminates the parametric  $q_{105}$  and  $q_{107}$ )
2.  $f_{ijk} \mapsto \frac{1}{f_{ijk}}$  (and removing the denominator in  $Q$  afterwards)
3.  $f_{ijk} \mapsto f_{ijk} - 1$ .

This produces the simplified form

$0 = Q = f_{001}f_{010}f_{100}f_{111} + f_{000}f_{011}f_{101}f_{110}$  that can be linearized:  
 $\log(-\dots) = \log(\dots)$  showing that the solution is trivial.

# The Solution with (— — —) Symmetry

## Main result:

The following is the only *non-trivial* 3d affine linear face formula with cubical symmetry that is 4d consistent:

$$Q = (f_{100} - f_{001})(f_{010} - f_{111})(f_{101} - f_{110})(f_{011} - f_{000}) - (f_{001} - f_{010})(f_{111} - f_{100})(f_{000} - f_{101})(f_{110} - f_{011}). \quad (1)$$

This is the discrete Schwarzian bi-Kadomtsev-Petviashvili system (dBKP-system) — an integrable discrete system (Nimmo, Schief (1998) and Konopelchenko, Schief (2002)). It appears in many different contexts.

# Outline

Discrete Differential Geometry

3d Faces that are 4d Consistent

Difficulties

Simplifications

    Cubical Symmetry

    Probing

Filling Holes by Digging new Ones

Solutions

**Parallelization of the Computation**

    Guidance Principles

    Overall Structure

    Case Splitting

    Flexibility

    Safety

    To Do

# Guidance Principles I

- ▶ Parallel computer algebra is hardly justified by a single application → aim at producing more generally applicable parallel programs together with the application.

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# Guidance Principles I

- ▶ Parallel computer algebra is hardly justified by a single application → aim at producing more generally applicable parallel programs together with the application.
- ▶ Parallelization should be flexible wrt. available hardware which is expensive and designed for numerical computations in batch mode and not for doing symbolic computations interactively.
- ▶ The effort in exchanging symbolic expressions is considerably large because a tree of cells linked through pointers has to be packed into a linear data structure, to be communicated and then to be unpacked. Therefore substantial subroutines leading to coarse grain parallelism should be parallelized first.

## Guidance Principles II

- ▶ The purpose of parallel computer algebra is to do large computations but large computations carry the risk of an explosion of the size of expressions, therefore for parallel CA extra precautions should be made to be save against too strong expression swell.

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- ▶ The purpose of parallel computer algebra is to do large computations but large computations carry the risk of an explosion of the size of expressions, therefore for parallel CA extra precautions should be made to be save against too strong expression swell.
- ▶ The more CPUs/nodes are involved in a single computation and the longer computations take (days, weeks or even longer) the more fault tolerant the whole setup has to be against hardware failure and partial or total system shut downs.

# Overall Structure

Computations are done with the package CRACK running under (Parallel) REDUCE. All features discussed below apply to the solving of any system (algebraic, ODEs, PDEs).

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Parallelization is currently restricted to a parallel investigation of the different cases and subcases (for algebraic and differential problems). This is the most coarse grain parallelization possible.

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- ▶ by considering a separant in a differential equation to be zero or not in order to do a reduction in a differential Gröbner basis computation, or
- ▶ by considering the most often occurring factor in a system of equations to be zero or non-zero (but only factors which if set to zero yield substitutions).

# Flexibility

## **Available hardware:**

several clusters of the SHARCNET consortium with, for example, 128 Itanium2 CPUs, 256 GB (silky), 384 Opteron CPUs (bull) or 3072 CPU (whale) running in batch mode and being very expensive with the need to be utilized fully.

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- ▶ automatic job submissions and automatic completion check

# Parallelization Techniques

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- ▶ *harder problems* needing occasional manual interference: parallelization within the environment of the Unix command screen
- ▶ *very tough problems*: duplication of process into another `xterm` window for a risk free interactive exploration

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- ▶ shortening algorithm
- ▶ time limits on any (time) risky modules, like factorization
- ▶ capture of all interactive input re-usable to restore an environment

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- ▶ parallel implementation of the shortening of equations
- ▶ competitive parallelism: different methods trying in parallel to make progress with a hard, large system
- ▶ more applications which will show new needs for improvements on probably many fronts (safety, optimal usage of hardware, documentation like online parallel tutorial, ...)