3-dim. scalar discrete integrable equations - an application for parallel CA

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

Introduction

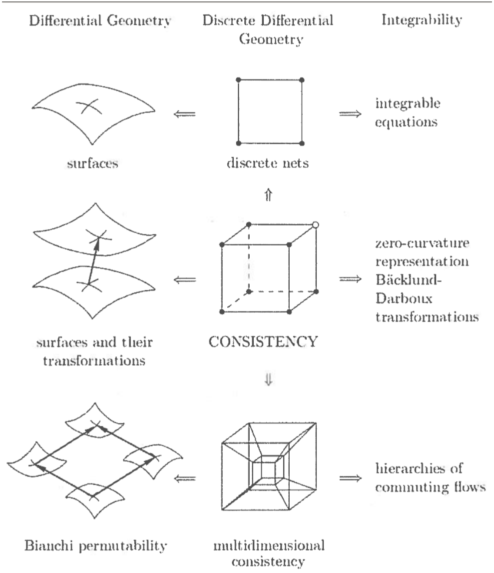
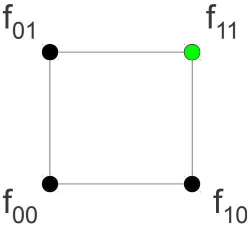


Figure 0.2. The consistency principle of discrete differential geometry as conceptual basis of the differential geometry of special surfaces and of integrability.

2d Faces



The object of interest is an affine linear relation

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

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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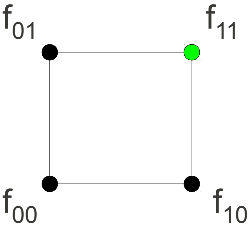

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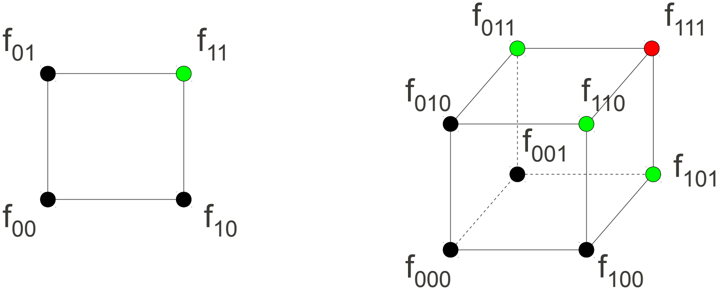
Of interest are such relations, i.e. values of coefficients $q_0, \ldots, q_{15}$, which are *3d consistent* in the following sense.

Consistency of 2d Face Relations



Example of a 2d face relation that is 3d consistent:
$f_{00}f_{11} - f_{01}f_{10} = 0$

The Consistence Condition

Using the face relation 6 times for the 6 squares of the surface of a cube with values $f_{000}, f_{001}, ..., f_{111}$ associated with the corners, the following must hold.

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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 $f_{000}, f_{001}, f_{010}, f_{100}$.
- This gives polynomial conditions for the unknown coefficients $q_0, .., q_{15}$ which have to be satisfied identically in the black corner values $f_{000}, f_{001}, f_{010}, f_{100}$.

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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, (2007) arXiv:0706.2464, Lett. in Math. Phys. DOI:10.1007/s11005-008-0230-2.

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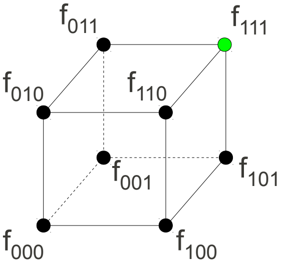

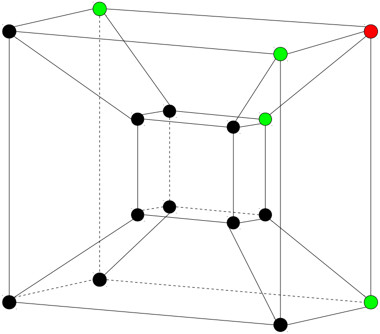

A 3d face relation that is 4d consistent:

$$0 = (f_{100}-f_{001})(f_{010}-f_{111})(f_{101}-f_{110})(f_{011}-f_{000}) - (f_{001}-f_{010})(f_{111}-f_{100})(f_{000}-f_{101})(f_{110}-f_{011})$$

(discrete Schwarzian bi-Kadomtsev-Petviashvili system)

The Setup

- **affine linearity of Q:**
  A 3d cube has $2^3 = 8$ corner values $f_{000}, f_{001}, \ldots, f_{111}$,

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

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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 $f_{0000}, f_{0001}, f_{0010}, \ldots, f_{1010}, f_{1100}$.
  - 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_α.

Outline

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	$2^{\{2^{n+1}(n+1)-2n-1\}}$	5.2×10^5	1.4×10^{17}	2.8×10^{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	$2n(2n+2)^{\left(2^{n+1}-n-3\right)}$	864	6.4×10^9	8.0×10^{25}
estimated average # of terms in each equation	$\frac{2^{2^{n+1}(n+1)-2n-1}}{2n(2n+2)^{\left(2^{n+1}-n-3\right)}}$	606	2.2×10^7	3.5×10^{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.

Outline

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	1 param.; 4 terms
	$(-+)$: 3 param.; 10 terms	none
	$(++)$: 6 param.; 16 terms	1 param.; 6 terms
3	$(---)$: 1 param.; 24 terms	1 param.; 24 terms
	$(-++)$: 13 param.; 186 terms	none
	$(+++)$: 22 param.; 256 terms	3 param.; 114 terms
4	$(----)$: 94 param.; 29208 terms	5 param.; 15480 terms
	$(+---)$: 77 param.; 26112 terms	none
	$(-+++)$: 349 param.; 60666 terms	3 param.; 15809 terms
	$(++++)$: 402 param.; 2^{16} 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
$f_\alpha : f_{0000}, f_{0001}, \ldots f_{1100}$ (with at most two 1's in the index).

- replace some ($:= z$) of the f_α by zero,
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- replace some ($:= u$) of the remaining f_α by a random integer $\neq 0$
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- keep the remaining $s := 11 - z - u$ variables f_α symbolic.

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- solve the remaining equations in the solution process.

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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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(–) As the computation splits into cases and $(\mathrm{sub}-)^{10-15}$cases the generated conditions are only valid in the corresponding case and its sub-cases $\rightarrow$ very many files of generated equations (e.g. too many to do in unix: `rm *`).

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(–) 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: $0 = A_k(f_\alpha)f_{1..101..1} + B_k(f_\alpha)$
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$\rightarrow$ 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 allows a parallel solution of (sub-)cases

Outline

Results

Case $(+++)$: 5 solutions

Case $(-++)$: 3 solutions

Case $(---)$: 1 solution

A Solution with $(+++)$ Symmetry

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

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: $\log(-...) = \log(...)$ 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:

$$\begin{aligned} Q = {} & (f_{100} - f_{001})(f_{010} - f_{111})(f_{101} - f_{110})(f_{011} - f_{000}) - \\ & (f_{001} - f_{010})(f_{111} - f_{100})(f_{000} - f_{101})(f_{110} - f_{011}). \end{aligned} \tag{1}$$

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

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- 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.

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- 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.

Case Splitting

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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 occuring 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

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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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- capture of all interactive input re-usable to restore an environment

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- more applications which will show new needs for improvements on probably many fronts (safety, optimal usage of hardware, documentation like online parallel tutorial, ...)