NIST

Electromagnetic Field Division Seminar

SYMBOLIC COMPUTING IN RESEARCH

Willy Hereman

Dept. of Mathematical and Computer Sciences
Colorado School of Mines
Golden, CO 80401-1887

Tuesday, March 10, 1992
10:30

Use of CAS in Electromagnetic Field Theory?

Bibliography of Publications referencing MACSYMA:

- Disk dynamos and magnetic reversal (1975)
- Rotating air gap armature machine as a superconducting induction motor for ship propulsion (1976)
- Transient electromagnetic fields over a two layer medium (1979)
- Microstrip capacitance for a circular disk (1980)
- 3D electric field solutions in boundary fitted coordinates (1983)
- Design of magnetic field coils (1984)
- Probing the earth with microwave remote sensing (1984)
- Analytical studies of electromagnetic problems with MACSYMA (1984)
- Relativistic electromagnetic instabilities near electron cyclotron frequency (1984)
- Electric field calculations for lasers (1984)

From: "Uses Made of Computer Algebra in Physics"
Cohen and Fitch, J. Sym. Comp. **11** (1991) 291-305:

- Quantum field theory and quantum gravity
- Evaluation of classes of Feynman diagrams (all loops)
- Decay rate of orthopositronium
  (quantum electro-dynamics)
- Single and two-channel Schrödinger equations
- Closed form expressions for Dirac-Coulomb
  radial integrals
- Ideal-gas-base low-density expansions
- Calculation of multiple covariant derivatives of orders
  7 and 8 (geodesic interval for Riemannian surfaces)
- N-bubble diagrams for leptonic g-2

I. INTRODUCTION

Review of Symbolic Manipulation Programs (CAS)

- MACSYMA (MIT, 1970; National Energy Software Center, Symbolics Inc., 1982) $ 1950
- MATHEMATICA (SMP, Interference Corp., 1970; Wolfram Research Inc., 1988) $ 495 - $ 695 (bundled with NeXT)
- MAPLE (Waterloo Maple Software Inc., 1980) $ 625
- REDUCE (Anthony Hearn, RAND Corporation, 1970) $ 495
- DERIVE (muMATH, 1970; Soft Warehouse Inc., 1988) $ 195
- AXIOM (Scratchpad II, IBM Research Center, 1970; NAG Library, 1991) $ 700
- Microcalc, MathCAD, Mathscribe, Cayley, GAP, MaCaulay, PowerMath, Scolar, Milo, etc. <$ 500

Sources of information

- Computer Algebra Conferences
  (SIGSAM, ACM, SAME)
- Computer Algebra Support Projects

- Offering Master's and Ph.D Projects:
  Kent State, University of Cantabria
  (Symbolic Computation under CS)
  Berkeley, Cambridge, Delaware, Bath, Liverpool
  Grenoble, Strasbourg, Paris, Nice, Ecole
  Polytechnique, Stockholm, London, Paderborn
  Aachen, Golden
- Research Institute for Symbolic Computation
  J. Kepler University, Linz, Austria
- Center for Symbolic Methods in Algorithmic
  Mathematics (MSI, Cornell University)
- Special courses: Modeling using MATHEMATICA
  CSM, Fall 1992
  Universities of Montréal, Drexel, Denver, etc.

- Journal of Symbolic Computation
- SIGSAM Bulletin of the ACM
- Macsyma Newsletter
- CASE, Maple, Mathematica & Macsyma Newsletters
- Electronic Mail discussion groups:
  Reduce, Mathematica, & Maple fora
- USENET
- Software Libraries: Reduce Library
  Computer Physics Communications Program Library
- Books on the subject: Mathematica (12), Macsyma (8), Maple (6), Reduce (6), Derive (6), muMATH (3), SMP (3)
- Numerous review articles
- On-line help, Interactive tutorials
- Primer Manuals, Reference Manuals, User Guides, Bibliographies of Applications, etc.

Why use computer algebra systems?

- quick and correct way of deriving exact, analytical results
- relieves the researcher from tedious and/or routine calculations
- leads to exploration of new ideas
- leads to new results
- development of new algorithms (programming)
- splendid post-calculation numerics and graphics
- detect errors in scientific literature (tables of integrals, 15 % , research papers, 30 %)
- effective teaching and research tool
- output in Fortran, C and page-makeup in TeX

How to use symbolic manipulation programs?

- THINK first (exponential expression swell)
- with care and caution (BUGS)
- know the mathematics behind the algorithm
- test cases: from easy to difficult
- use different systems simultaneously
- work in batch mode (not interactively)
- avoid long expressions
- tricks, experience, practice, etc.
- use the graphical capabilities

Warm-up demonstration with MACSYMA

- Factorization of expressions
- Determinant and inverse of a Vandermonde matrix
- Inverse of the Hilbert matrix
- Sums (powers of integers) and products (Wallis Π product)
- Differentiation and integration
- Solving differential equations
- Special functions (Bessel & Error functions)
- Roots via polynomial decomposition

II. **SYMBOLIC MANIPULATION in RESEARCH**

- Soliton phenomenon (Mathematica)
- Dependency on parameters (Macsyma)
- Software programs for Soliton Theory (Macsyma)
  - Painlevé integrability test for single ODE or PDE
  - Lie point symmetries of systems of PDEs
  - Solitary waves via real exponential approach
  - Construction of soliton solutions (Hirota's method)
- Taylor expansions and approximations (Derive)

Example 1 – Macsyma
Exact Solutions of Nonlinear PDEs

- Hirota's Direct Method
  allows to construct exact soliton solutions of
  - nonlinear evolution equations
  - wave equations
  - coupled systems
- Test conditions for existence of soliton solutions
- Examples:
  - Korteweg-de Vries equation (KdV)

$$u_t + 6uu_x + u_{3x} = 0$$

  - Kadomtsev-Petviashvili equation (KP)

$$(u_t + 6uu_x + u_{3x})_x + 3u_{2y} = 0$$

  - Sawada-Kotera equation (SK)

$$u_t + 45u^2u_x + 15u_xu_{2x} + 15uu_{3x} + u_{5x} = 0$$

Hirota's Method

Korteweg-de Vries equation

$$u_t + 6uu_x + u_{3x} = 0$$

Substitute

$$u(x,t) = 2\frac{\partial^2 \ln f(x,t)}{\partial x^2}$$

Integrate with respect to x

$$f\,f_{xt} - f_x f_t + f\,f_{4x} - 4f_x f_{3x} + 3f_{2x}^2 = 0$$

Bilinear form

$$B(f{\cdot}f) \stackrel{\text{def}}{=} \left(D_x D_t + D_x^4\right)(f{\cdot}f) = 0$$

Introduce the bilinear operator

$$D_x^m\,D_t^n(f{\cdot}g) = (\partial x - \partial x')^m(\partial t - \partial t')^n f(x,t)\,g(x',t')|_{x'=x,t'=t}$$

Use the expansion

$$f = 1 + \sum_{n=1}^{\infty} \epsilon^n\, f_n$$

Substitute f into the bilinear equation

Collect powers in ϵ (book keeping parameter)

$$O(\epsilon^0)\ :\ B(1{\cdot}1) = 0$$

$$O(\epsilon^1)\ :\ B(1{\cdot}f_1 + f_1{\cdot}1) = 0$$

$$
\begin{aligned}
O(\epsilon^2) &: B(1{\cdot}f_2 + f_1{\cdot}f_1 + f_2{\cdot}1) = 0 \\
O(\epsilon^3) &: B(1{\cdot}f_3 + f_1{\cdot}f_2 + f_2{\cdot}f_1 + f_3{\cdot}1) = 0 \\
O(\epsilon^4) &: B(1{\cdot}f_4 + f_1{\cdot}f_3 + f_2{\cdot}f_2 + f_3{\cdot}f_1 + f_4{\cdot}1) = 0 \\
O(\epsilon^n) &: B(\sum_{j=0}^{n} f_j{\cdot}f_{n-j}) = 0 \qquad \text{with } f_0 = 1
\end{aligned}
$$

If the original PDE admits a N-soliton solution
then the expansion will truncate at level $n = N$ provided

$$f_1 = \sum_{i=1}^{N} \exp(\theta_i) = \sum_{i=1}^{N} \exp\left(k_i\, x - \omega_i\, t + \delta_i\right)$$

k_i, ω_i and δ_i are constants

Dispersion law

$$\omega_i = k_i^3 \qquad (i = 1, 2, ..., N)$$

Consider the case N=3
Terms generated by $B(f_1, f_1)$ justify

$$
\begin{aligned}
f_2 &= a_{12}\, \exp(\theta_1 + \theta_2) + a_{13}\, \exp(\theta_1 + \theta_3) + a_{23}\, \exp(\theta_2 + \theta_3) \\
&= a_{12}\, \exp\left[(k_1 + k_2)\, x - (\omega_1 + \omega_2)\, t + (\delta_1 + \delta_2)\right] \\
&+ a_{13}\, \exp\left[(k_1 + k_3)\, x - (\omega_1 + \omega_3)\, t + (\delta_1 + \delta_3)\right] \\
&+ a_{23}\, \exp\left[(k_2 + k_3)\, x - (\omega_2 + \omega_3)\, t + (\delta_2 + \delta_3)\right]
\end{aligned}
$$

Calculate the constants a_{12}, a_{13} and a_{23}

$$a_{ij} = \frac{(k_i - k_j)^2}{(k_i + k_j)^2} \qquad i, j = 1, 2, 3$$

$B(f_1 \cdot f_2 + f_2 \cdot f_1)$ motivates

$$\begin{aligned} f_3 &= b_{123} \exp(\theta_1 + \theta_2 + \theta_3) \\ &= b_{123} \exp\left[(k_1 + k_2 + k_3)x - (\omega_1 + \omega_2 + \omega_3)t + (\delta_1 + \delta_2 + \delta_3)\right] \end{aligned}$$

with

$$b_{123} = a_{12}\, a_{13}\, a_{23} = \frac{(k_1 - k_2)^2 (k_1 - k_3)^2 (k_2 - k_3)^2}{(k_1 + k_2)^2 (k_1 + k_3)^2 (k_2 + k_3)^2}$$

Subsequently, $f_i = 0$ for $i > 3$

Set $\epsilon = 1$

$$\begin{aligned} f &= 1 + \exp\theta_1 + \exp\theta_2 + \exp\theta_3 \\ &+ a_{12} \exp(\theta_1 + \theta_2) + a_{13} \exp(\theta_1 + \theta_3) + a_{23} \exp(\theta_2 + \theta_3) \\ &+ b_{123} \exp(\theta_1 + \theta_2 + \theta_3) \end{aligned}$$

Return to the original $u(x, t)$

$$u(x, t) = 2 \frac{\partial^2 \ln f(x, t)}{\partial x^2}$$

Single soliton solution

$$f = 1 + e^{\theta}\ , \qquad \theta = kx - \omega t + \delta$$

k, ω and δ are constants and $\omega = k^3$

Substituting f into

$$\begin{aligned} u(x,t) &= 2\frac{\partial^2 \ln f(x,t)}{\partial x^2} \\ &= 2(\frac{f_{xx}f - f_x^2}{f^2}) \end{aligned}$$

Take $k = 2K$

$$u = 2K^2 \text{sech}^2 K(x - 4K^2 t + \delta)$$

Two-soliton solution

$$f = 1 + e^{\theta_1} + e^{\theta_2} + a_{12}e^{\theta_1+\theta_2}$$

$$\theta_i = k_i x - \omega_i t + \delta_i$$

with $\omega_i = k_i^3$, $(i = 1, 2)$ and $a_{12} = \frac{(k_1-k_2)^2}{(k_1+k_2)^2}$

Select

$$\begin{aligned} e^{\delta_i} &= \frac{c_i^2}{k_i} e^{k_i x - \omega_i t + \Delta_i} \\ \tilde{f} &= \frac{1}{4} f e^{-\frac{1}{2}(\tilde{\theta}_1+\tilde{\theta}_2)} \\ \tilde{\theta}_i &= k_i x - \omega_i t + \Delta_i \\ c_i^2 &= \left(\frac{k_2+k_1}{k_2-k_1}\right) k_i \end{aligned}$$

Return to $u(x, t)$

$$\begin{aligned} u(x,t) &= \tilde{u}(x,t) = 2\frac{\partial^2 \ln \tilde{f}(x,t)}{\partial x^2} \\ &= \left(\frac{k_2^2 - k_1^2}{2}\right)\left(\frac{k_2^2 \text{cosech}^2 \frac{\tilde{\theta}_2}{2} + k_1^2 \text{sech}^2 \frac{\tilde{\theta}_1}{2}}{(k_2 \coth \frac{\tilde{\theta}_2}{2} - k_1 \tanh \frac{\tilde{\theta}_1}{2})^2}\right) \end{aligned}$$

Example 2 – Mathematica
Soliton Interaction

Korteweg-de Vries equation

$$u_t + 6uu_x + u_{3x} = 0$$

Take a four soliton solution

$$\begin{aligned} u(x,t) &= 2\frac{\partial^2 \ln f(x,t)}{\partial x^2} \\ &= 2\left(\frac{f_{xx}f - f_x^2}{f^2}\right) \end{aligned}$$

generated by

$$f = 1 + e^{\theta_1} + e^{\theta_2} + e^{\theta_3} + e^{\theta_4} + a_{12} + e^{\theta_1+\theta_2} + \cdots$$

with $\theta_i = k_i\, x - k_i^3\, t + \delta_i \qquad (i = 1, 2, 3, 4)$

Select $k_1 = 8, k_2 = 64, k_3 = 216, k_4 = 512$

and δ_i such that $u(x, 0) = 20\,\mathrm{sech}^2\, x$

Plot $u(x,t)$ as function of x for various values of t

Animate the result

Example 3 – Macsyma
Painlevé Integrability Test

Integrability of a PDE requires that the only **movable singularities** in its solution are **poles**

Singularities are **movable** if their location depends on the initial conditions

Critical points (including logarithmic branch points and essential singularities) must be fixed to have integrability

Definition: A simple equation or system has the *Painlevé Property* if its solution in the complex plane has no worse singularities than movable poles

Aim: Verify if the PDE satisfies the **necessary criteria** to have the *Painlevé Property*

The solution f expressed as a Laurent series,

$$f = g^{\alpha} \sum_{k=0}^{\infty} u_k g^k$$

should only have movable poles

$u_0(t,x) \neq 0$, α is a negative integer
$u_k(t,x)$ are analytic functions in a neighborhood of the singular, non-characteristic manifold $g(t,x) = 0$, with $g_x(t,x) \neq 0$

Steps of the Painlevé Test

- **Step 1**:
  1. Substitute the **leading order** term,
  $$f \propto u_0 \, g^\alpha$$
  into the given equation
  2. Determine the integer $\alpha < 0$ by balancing the most singular terms in g
  3. Calculate u_0
- **Step 2**:
  1. Substitute the generic terms
  $$f \propto u_0 \, g^\alpha + u_r \, g^{\alpha+r}$$
  into the equation, retaining its most singular terms
  2. Require that u_r is arbitrary
  3. Calculate the corresponding values of $r > 0$, called **resonances**

- **Step 3**:
  1. Substitute the truncated expansion
  $$f = g^{\alpha} \sum_{k=0}^{R} u_k \, g^k, \tag{4}$$
  where R represents the largest resonance, into the complete equation
  2. Determine u_k unambiguously at the non-resonance levels
  3. Check whether or not the **compatibility condition** is satisfied at resonance levels

- An equation or system has the **Painlevé Property** and is conjectured to be integrable if:
  1. Step 1 thru 3 can be carried out consistently with $\alpha < 0$ and with positive resonances
  2. The compatibility conditions are identically satisfied for all resonances

- For an equation to be integrable it is **necessary** but **not sufficient** that it passes the Painlevé test
- The above algorithm does not detect the existence of essential singularities

Demo Painlevé Test

Korteweg-de Vries equation

$$u_t + 6uu_x + u_{3x} = 0$$

Example 4 – Macsyma
Positioning of Equipment

A Trilateration Problem

Calculate the unknown 3D-position of a point,
given the distances from that point to a set of fixed points

x and y are the horizontal coordinates
z is the altitude of the unknown point

Questions:

- Is there a mathematical solution?
- What is the smallest number of beacons needed?
- Can the position of the bulldozer be determined "fairly accurately" if the distances are inaccurate?
- What are the optimal positions of the beacons?
- What is the 'best' optimal algorithm for the solution?
- Can the algorithm be translated into a fast C-program?
- What are the possible applications of the problem?

A Mathematical Solution

Linearization

(x_i, y_i, z_i) $(i = 1, 2, ..., n)$ are the known coordinates of the n beacons

(x, y, z) are the unknown coordinates of the bulldozer

r_i are *measured* approximate slope distances from bulldozer to beacons

Constraints

$$(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2 = {r_i}^2$$

Use the j^{th} constraint as a *linearizing* tool

Add and subtract x_j, y_j and z_j

$$(x - x_j + x_j - x_i)^2 + (y - y_j + y_j - y_i)^2 + (z - z_j + z_j - z_i)^2 = {r_i}^2$$

Expand and regroup terms

$$\begin{aligned}
&(x - x_j)(x_i - x_j) + (y - y_j)(y_i - y_j) + (z - z_j)(z_i - z_j) \\
&= \frac{1}{2}[(x - x_j)^2 + (y - y_j)^2 + (z - z_j)^2 \\
&\quad - {r_i}^2 + (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2]
\end{aligned}$$

$$= \frac{1}{2}[{r_j}^2 - {r_i}^2 + d_{ij}^2]$$

where

$$d_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

is the distance between beacons i and j

Select $j = 1$, thus for $i = 2, 3, ..., n$
linear system of $(n - 1)$ eqs. in 3 unknowns:

$$(x - x_1)(x_2 - x_1) + (y - y_1)(y_2 - y_1) + (z - z_1)(z_2 - z_1)$$
$$= \frac{1}{2}[{r_1}^2 - {r_2}^2 + d_{21}^2] = b_{21}$$

$$(x - x_1)(x_3 - x_1) + (y - y_1)(y_3 - y_1) + (z - z_1)(z_3 - z_1)$$
$$= \frac{1}{2}[{r_1}^2 - {r_3}^2 + d_{31}^2] = b_{31}$$

$$\vdots$$

$$(x - x_1)(x_n - x_1) + (y - y_1)(y_n - y_1) + (z - z_1)(z_n - z_1)$$
$$= \frac{1}{2}[{r_1}^2 - {r_n}^2 + d_{n1}^2] = b_{n1}$$

In matrix form $A\vec{x} = \vec{b}$, with

$$A = \begin{pmatrix} x_2 - x_1 & y_2 - y_1 & z_2 - z_1 \\ x_3 - x_1 & y_3 - y_1 & z_3 - z_1 \\ \vdots & \ddots & \vdots \\ x_n - x_1 & y_n - y_1 & z_n - z_1 \end{pmatrix}$$

$$\vec{x} = \begin{pmatrix} x - x_1 \\ y - y_1 \\ z - z_1 \end{pmatrix}, \qquad \vec{b} = \begin{pmatrix} b_{21} \\ b_{31} \\ \vdots \\ b_{n1} \end{pmatrix}$$

The Least Squares Method

The distances r_i are only approximate
Determine $\vec{x}$ such that $A\vec{x} \approx \vec{b}$

Minimize the sum of the squares of the residuals

$$S = \vec{r}^{\,T}\vec{r} = (\vec{b} - A\vec{x})^T (\vec{b} - A\vec{x})$$

Solve the *normal* equation

$$A^T A\vec{x} = A^T\vec{b}$$

If $A^T A$ is non-singular then

$$\vec{x} = (A^T A)^{-1} A^T \vec{b}$$

Determine the effect of adding errors to the radii

Demo with the actual data from the coal mine