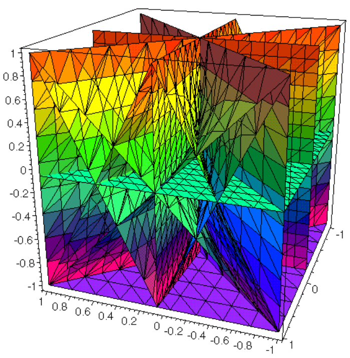
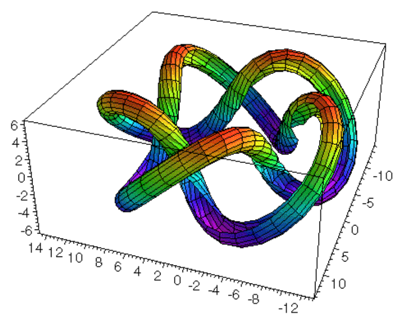
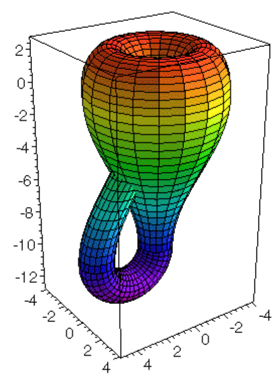
Computer Algebra at Work







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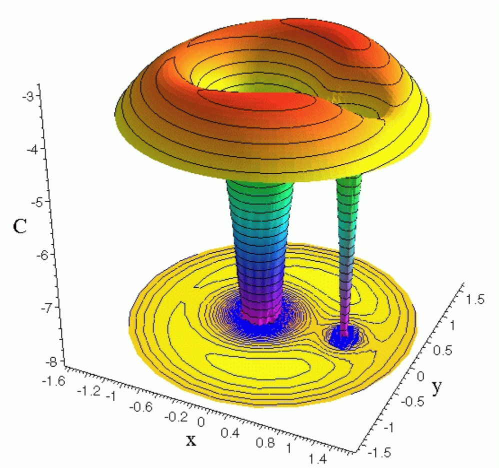
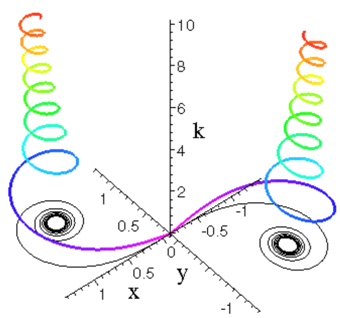




What Is Computer Algebra?

- Generation and manipulation of algebraic expressions using a computer. This includes a vast selection of mathematical topics.
- algebraic computations
  - expanding, factoring, simplifying
  - solving equations & systems of equations
- calculus
  - differentiation
  - integrals
  - series expansions
  - limits

What Is Computer Algebra? (continued)

- linear algebra
  - matrix algebra
  - eigenvalues and eigenvectors
- ODEs

$$\left(\frac{\partial^2}{\partial\theta\,\partial\theta}x\right) - 2\left(\frac{\partial}{\partial\theta}y\right) = \frac{\partial}{\partial x}\Omega$$

$$\left(\frac{\partial^2}{\partial\theta\,\partial\theta}y\right) + 2\left(\frac{\partial}{\partial\theta}x\right) = \frac{\partial}{\partial y}\Omega$$

$$\left(\frac{\partial^2}{\partial\theta\,\partial\theta}z\right) + z = \frac{\partial}{\partial z}\Omega$$

$$\Omega = h\left(\frac{x^2+y^2+z^2}{2} + \frac{1-\mu}{r_1} + \frac{\mu}{r_2}\right)$$

$$r_1 = \sqrt{(x+\mu\,R)^2+y^2+z^2}$$

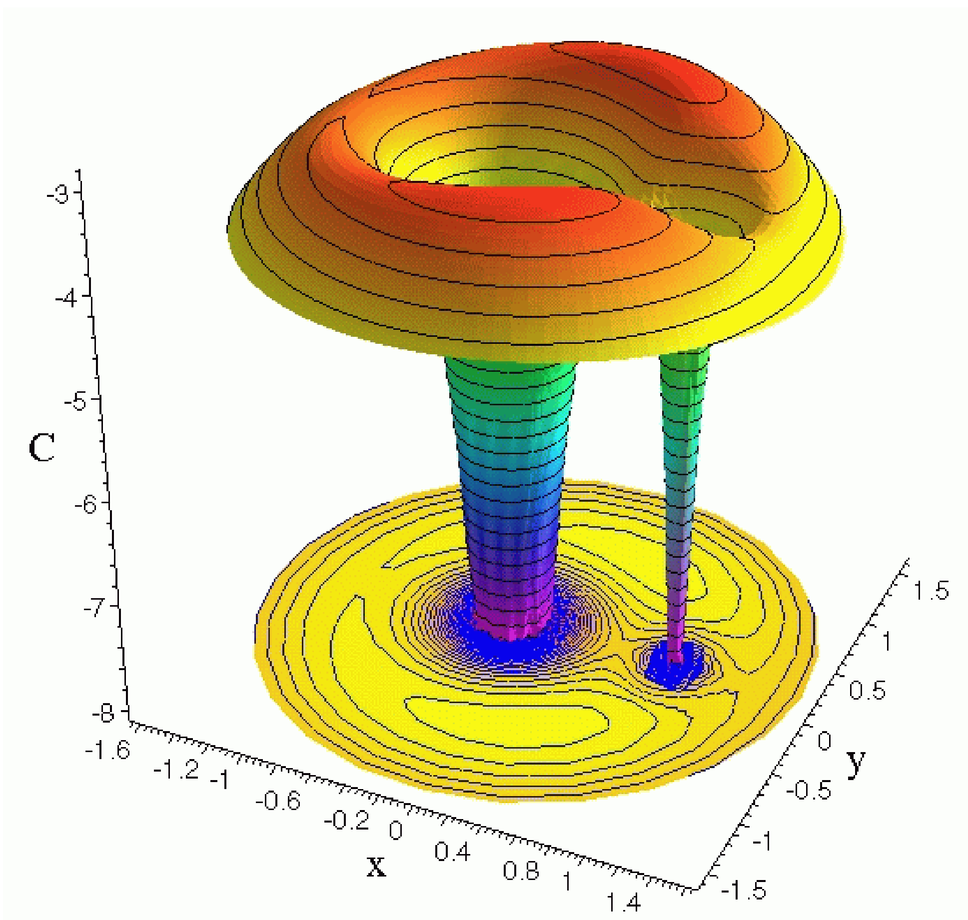
$$r_2 = \sqrt{(x-(1-\mu)\,R)^2+y^2+z^2}$$

$$R = h\,(1-e^2)$$

$$h = \frac{1}{1+e\cos(\theta)}$$

What Is Computer Algebra? (continued)

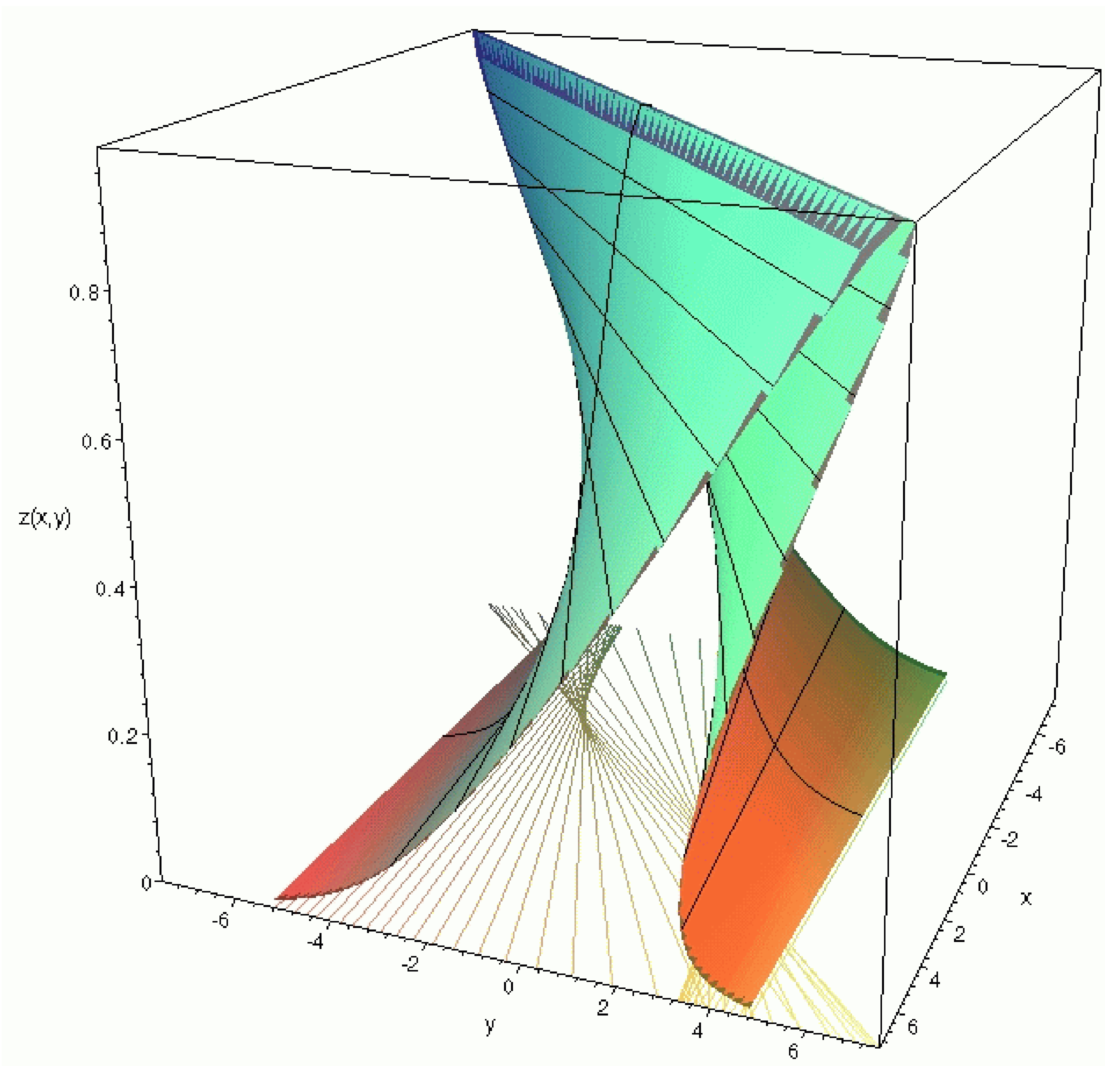
- Plot an invariant surface:



What Is Computer Algebra? (continued)

- PDEs

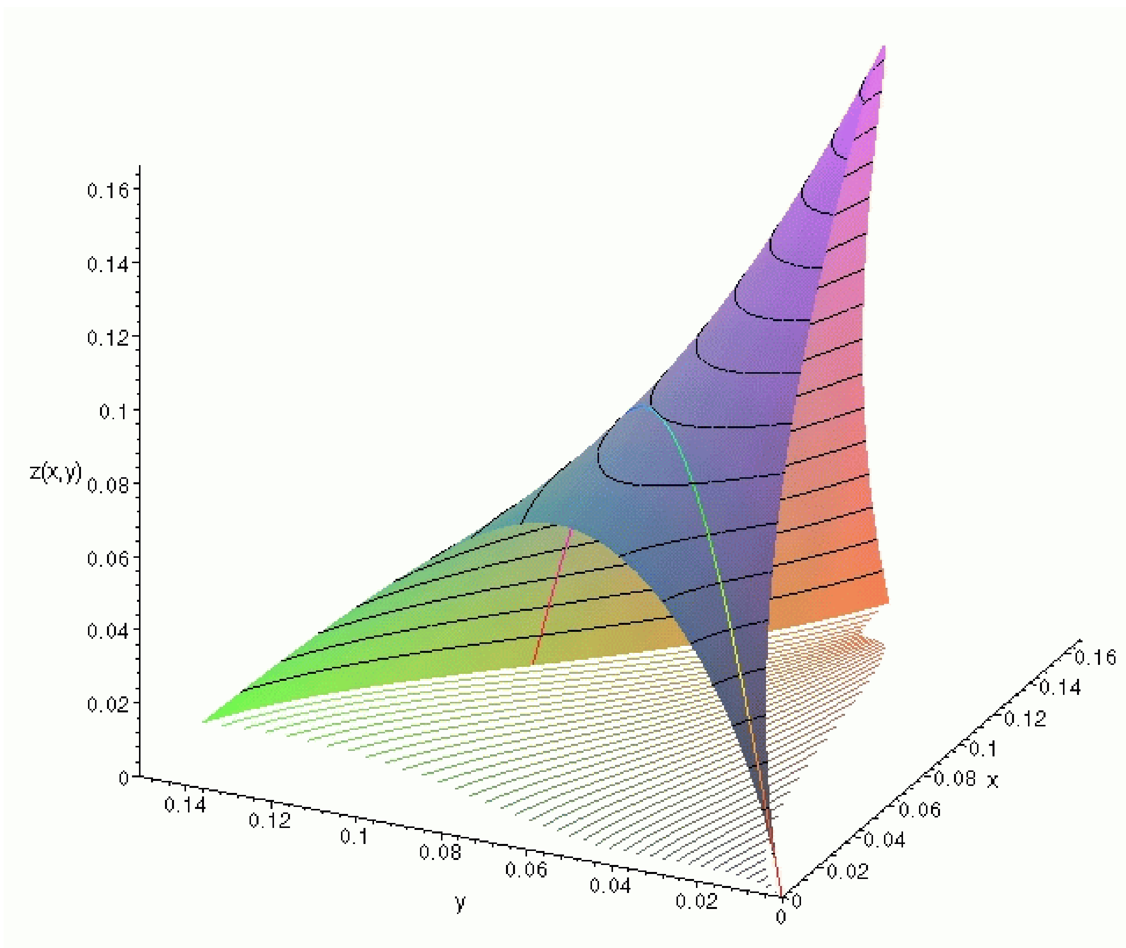
$$\left(\frac{\partial}{\partial x}\mathrm{z}(x,y)\right)+\mathrm{z}(x,y)\left(\frac{\partial}{\partial y}\mathrm{z}(x,y)\right)=0$$



What Is Computer Algebra? (continued)

- PDEs

$$\left(y^2 + z(x,y)^2 + x^2\right)\left(\frac{\partial}{\partial x} z(x,y)\right) - 2\,x\,y\left(\frac{\partial}{\partial y} z(x,y)\right) - 2\,z(x,y)\,x = 0$$



What Is Computer Algebra? (continued)

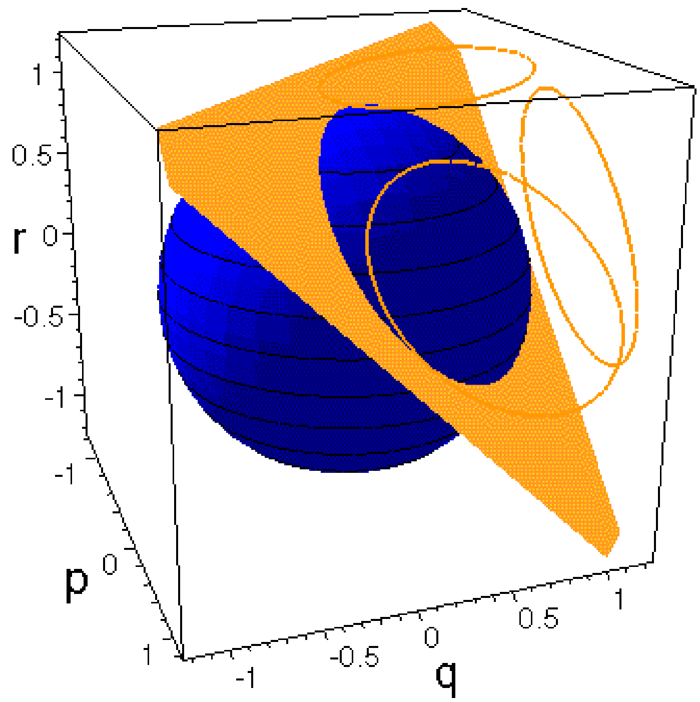
- numerical calculations
  - arbitrary digit precision

```
π = 3.14159265358979323846264338327950288419716939937510
      5820974944592307816406286208998628034825342117067982
      1480865132823066470938446095505822317253594081284811
      1745028410270193852110555964462294895493038196442881
      0975665933446128475648233786783165271201909145648566
      9234603486104543266482133936072602491412737245870066
      0631558817488152092096282925409171536436789259036001
      1330530548820466521384146951941511609433057270365759
      5919530921861173819326117931051185480744623799627495
      673518857527248912279381830119491
```

- statistics
  - Mean, Median, Variance, and Standard Deviation
  - least squares
  - probability distributions
- graphics
  - 2D plots
  - 3D plots (surfaces, space curves)
  - implicit plotting
  - animation

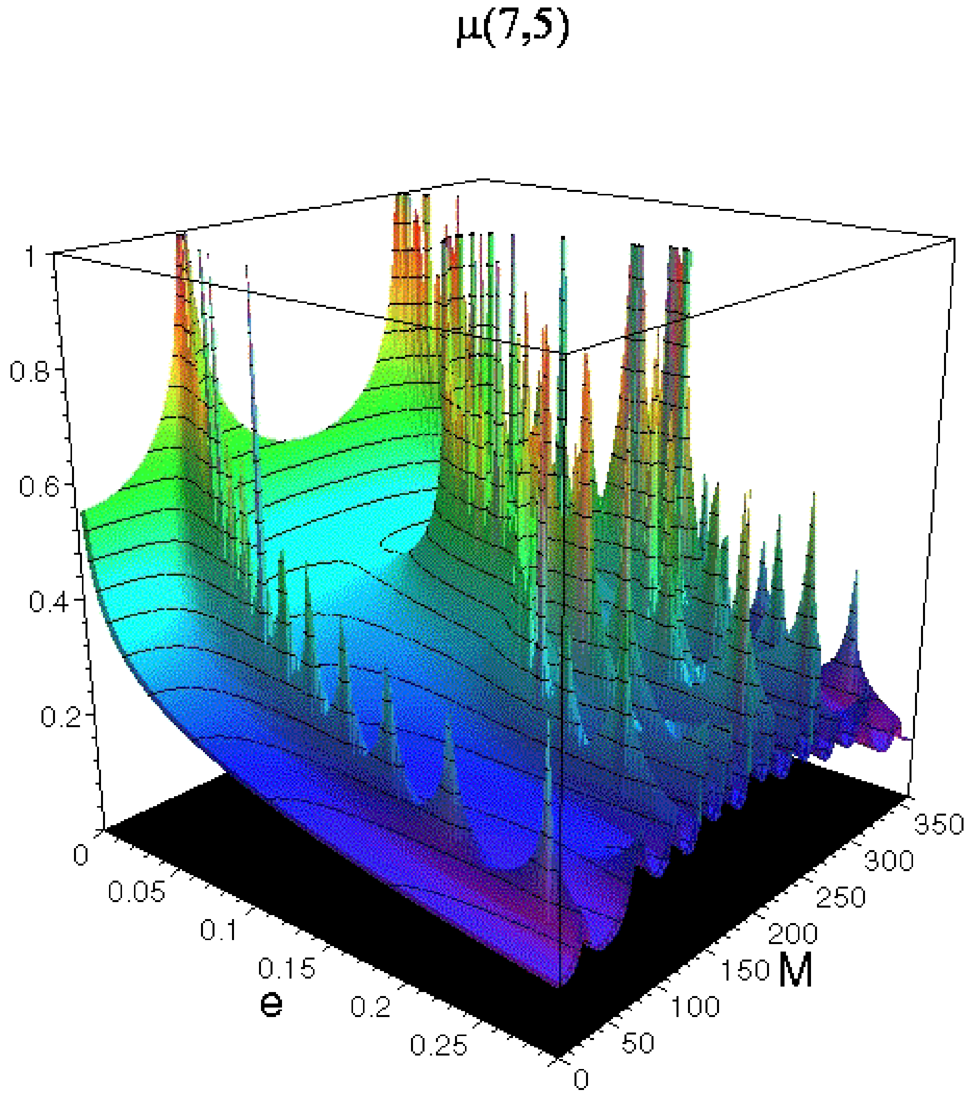
What Is Computer Algebra? (continued)

- 3D graphics example: Constraints in a Kasner Universe (a particular solution to General Relativity equations)



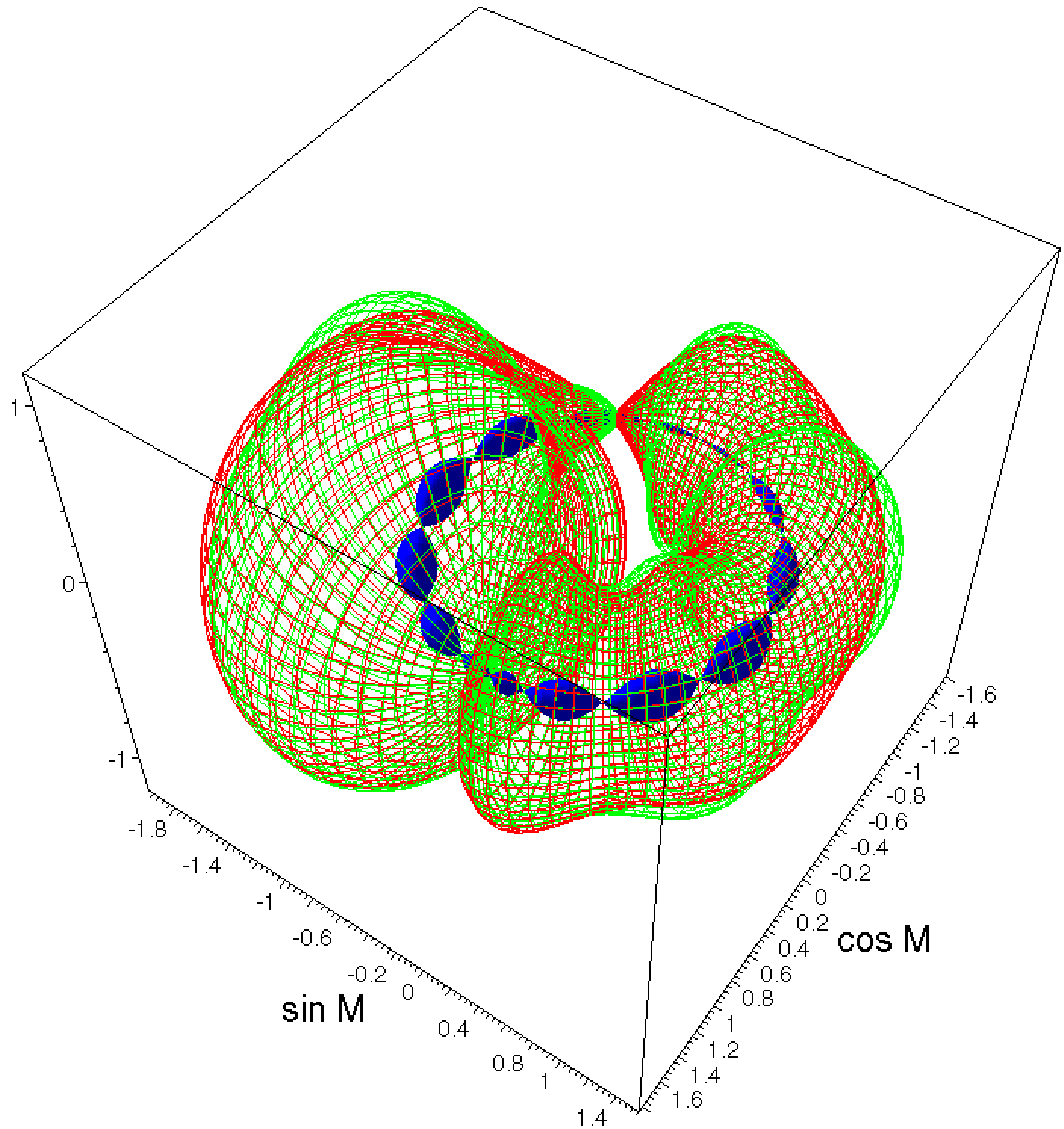
What Is Computer Algebra? (continued)

- 3D graphics example: Maximum tolerated time span for a series approximation of Keplerian motion



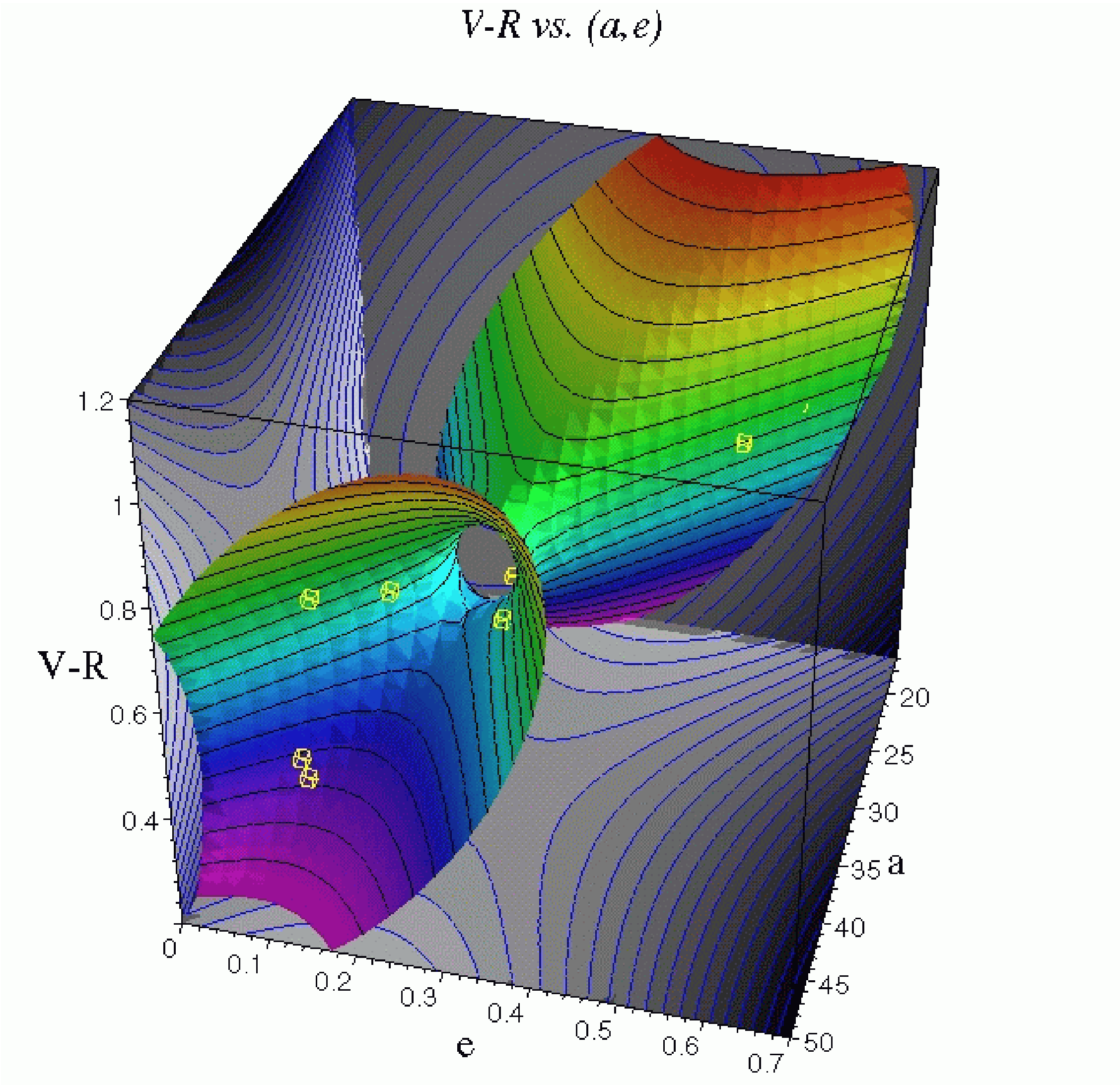
What Is Computer Algebra? (continued)

- 3D graphics example: Series approximation errors of different expansions of Keplerian motion



What Is Computer Algebra? (continued)

- 3D graphics example: Color (V-R) data for trans-Neptunian objects, with a least squares quadric surface fit



What Is Computer Algebra? (continued)

- programming — symbolic procedures

Maple V Release 5 - [KeplerSolve.mws]

$Keq := \phi = e\sin(\phi) + M$

$N := 6$

```
phi[0]=M;
for j to N do
  phi[j] = subs(phi=rhs(%),rhs(Keq));
  subs( f=phi, expansion( subs(phi=f,%), e, j ) );
  collect(combine(%,trig),e);
  print(%)
od:
```

$$\phi_0 = M$$

$$\phi_1 = e\sin(M) + M$$

$$\phi_2 = M + e\sin(M) + \frac{1}{2}e^2\sin(2M)$$

$$\phi_3 = \left(\frac{3}{8}\sin(3M) - \frac{1}{8}\sin(M)\right)e^3 + \frac{1}{2}e^2\sin(2M) + e\sin(M) + M$$

$$\phi_4 = \left(\frac{1}{3}\sin(4M) - \frac{1}{6}\sin(2M)\right)e^4 + \left(\frac{3}{8}\sin(3M) - \frac{1}{8}\sin(M)\right)e^3 + \frac{1}{2}e^2\sin(2M) + e\sin(M) + M$$

$$\phi_5 = \left(-\frac{27}{128}\sin(3M) + \frac{1}{192}\sin(M) + \frac{125}{384}\sin(5M)\right)e^5 + \left(\frac{1}{3}\sin(4M) - \frac{1}{6}\sin(2M)\right)e^4 + \left(\frac{3}{8}\sin(3M) - \frac{1}{8}\sin(M)\right)e^3 + \frac{1}{2}e^2\sin(2M) + e\sin(M) + M$$

$$\phi_6 = \left(\frac{1}{48}\sin(2M) + \frac{27}{80}\sin(6M) - \frac{4}{15}\sin(4M)\right)e^6 + \left(-\frac{27}{128}\sin(3M) + \frac{1}{192}\sin(M) + \frac{125}{384}\sin(5M)\right)e^5 + \left(\frac{1}{3}\sin(4M) - \frac{1}{6}\sin(2M)\right)e^4 + \left(\frac{3}{8}\sin(3M) - \frac{1}{8}\sin(M)\right)e^3 + \frac{1}{2}e^2\sin(2M) + e\sin(M) + M$$

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What Is Computer Algebra? (continued)

Maple V Release 5 - [KeplerSolve.mws]

Another approach, which yields the same result, is to construct a trial solution in the form of a power series in eccentricity,

$$\phi = \sum_{n=0}^{N} C_n e^n$$

$$\phi = C_0 + C_1 e + C_2 e^2 + C_3 e^3 + C_4 e^4 + C_5 e^5 + C_6 e^6$$

Substitute this back into the Kepler equation and solve for the coefficients. Here is a Maple procedure that does this:

```
#---------------------------------------------------------------
# Solve an equation phi = F(phi,eps) by series expansion, where
# phi is the solution variable and eps is a small parameter.
#---------------------------------------------------------------
xsolve := proc( expr::{algebraic,algebraic=algebraic},
                soln_var::{name,function},
                small_param::name,
                expansion_order::posint )

  local k, eqn, sols, S, trial, C;

  if type(expr,`=`) then
    S := lhs(expr) - rhs(expr);
  else
    S := expr;
  fi;

  #Create a trial solution of the form
  #  phi = C[0] + C[1]*eps + ... + C[N]*eps^N
  #and substitute that into the equation, then
  #expand into a power series to order N.
  trial := sum( C[k]*small_param^k, k=0..expansion_order );
  subs( soln_var=trial, S );
  S := expansion( %, small_param, expansion_order );

  #Solve for the coefficients C[k], starting with C[0]
  #and successively working our way up to C[N], by equating
  #coefficients of like powers of eps to zero.
  sols := [];
  for k from 0 to expansion_order do
    coeff( S, small_param, k );
    eqn := isolate( subs(sols,%), C[k] );
    if nargs > 4 then
      eqn := args[5]( eqn, args[6..nargs] );
    fi;
    sols := [ op(sols), eqn ];
  od;

  soln_var = subs( sols, trial );

end:
```

Applying this to the Kepler equation, we find

xsolve(*Keq*, ϕ, *e*, *N*, *combine*, *trig*)

$$\phi = M + \sin(M)\,e + \frac{1}{2}\sin(2M)\,e^2 + \left(\frac{3}{8}\sin(3M) - \frac{1}{8}\sin(M)\right)e^3 + \left(-\frac{1}{6}\sin(2M) + \frac{1}{3}\sin(4M)\right)e^4 + \left(-\frac{27}{128}\sin(3M) + \frac{1}{192}\sin(M) + \frac{125}{384}\sin(5M)\right)e^5 + \left(\frac{1}{48}\sin(2M) + \frac{27}{80}\sin(6M) - \frac{4}{15}\sin(4M)\right)e^6$$

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What Is Computer Algebra? (continued)

- environment
  - worksheet interface
  - export fortran or C code
  - export documents to HTML and LaTeX

What Is Computer Algebra? (continued)

Maple V Release 5 - [KeplerSolve.mws]

File Edit View Insert Format Spreadsheet Options Window Help

Least Squares Fit and Determination of Chebyshev Series Coefficients

Let us write the truncation error for an order N approximation of $f(x)$:

$$\varepsilon_N = f(x) - \left(\sum_{k=0}^{N} a_k\, T_k(x)\right)$$

One measure of goodness of fit of a polynomial to a function is the least squares integral

$$S_N = \int_{-1}^{1} w(x)\, {\varepsilon_N}^2\, dx$$

for some weighting function $w(x)$. To minimize S_N, we set $\frac{\partial}{\partial a_k} S_N = 0$ for all the a_k, finding

$$\int_{-1}^{1} 2\, w(x) \left(f(x) - \left(\sum_{n=0}^{N} a_n\, T_n(x)\right)\right) T_k(x)\, dx = 0$$

Let the weighting function be $w(x) = \frac{1}{\sqrt{1-x^2}}$. Then

$$\sum_{n=0}^{N} a_n \int_{-1}^{1} \frac{T_n(x)\, T_k(x)}{\sqrt{1-x^2}}\, dx = \int_{-1}^{1} \frac{f(x)\, T_k(x)}{\sqrt{1-x^2}}\, dx$$

Using the orthogonality relations, we arrive at the results

$$\pi\, a_0 = \int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\, dx$$

and

$$\pi\, a_k = 2 \int_{-1}^{1} \frac{f(x)\, T_k(x)}{\sqrt{1-x^2}}\, dx \quad \text{for } k \neq 0$$

These are equivalent to

$$\pi\, a_0 = \int_{0}^{\pi} f(\cos\theta)\, d\theta$$

and

$$\pi\, a_k = 2 \int_{0}^{\pi} f(\cos\theta) \cos(k\,\theta)\, d\theta \quad \text{for } k \neq 0$$

where $\cos\theta = x$.

A Chebyshev Series Expansion

Determination of the Coefficients

Suppose we expand $\phi - M = e \sin\phi$ in a Chebyshev series:

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Where can I get Computer Algebra?

- The "Big Three" general packages:
  - Macsyma
    - http://www.macsyma.com/
    - $199-$349 (depending on options)
  - Maple
    - http://www.maplesoft.com/
    - $1,099 ($699 academic)
  - Mathematica
    - http://www.wolfram.com/
    - $1,495 (??? academic)

A Real-Life Example

- Evaluation of a photon sensitivity integral for a spacecraft (FAME) detector:

$$S(r,s,g,T,v_1,v_2)=\int_{v_1}^{v_2}\frac{\sin^2 sv\sin rv-\sin^2 rgv}{e^{\frac{hv}{kT}}-1}dv$$

- This integral is intractible, so use a series expansion as an approximation for the black body spectrum term:

$$\frac{1}{e^{\frac{hv}{kT}}-1}=\sum_k a_k v^{k-1}$$

- To fourth power in optical frequency, the integral we must solve becomes

$$S=\int_{v_1}^{v_2}(a_0+a_1x+a_2x^2+a_3x^3+a_4x^4)(\sin^2 sx\sin rx-\sin^2 rgx)\,dx$$

  which can be done via successive applications of integration by parts.

- We've now reduced our problem to a conceptually simple, but practically unpleasant, task. Hence, we turn to our Computer Algebra tool.

A Real-Life Example (continued)

- Lesson #1: ALWAYS CHECK YOUR RESULT!

3. Check of the Indefinite Integral

Differentiate the indefinite integration result and check that it is equal to the integrand.

$$gawdawfulness := \operatorname{expand}\left(\left(\frac{\partial}{\partial x}\operatorname{rhs}(indef)\right) - integrand_1\right)$$

cost(%)

$$5770\ additions + 27247\ multiplications + 2328\ divisions + 5754\ functions + 2243\ subscripts$$

$\operatorname{collect}(gawdawfulness, [\sin, \cos, \operatorname{seq}(a_k, k = 0 .. 4), x], factor)$

cost(%)

$$54\ additions + 174\ multiplications + 13\ functions + 55\ subscripts$$

factor(combine(%%))

$$0$$

Whew.

- Corollary: TRUST NOTHING!

A Real-Life Example (continued)

- Lesson #2: ALWAYS DO YOUR CALCULATION TWO DIFFERENT WAYS, IF POSSIBLE!

5. Comparison between Definite and Indefinite Integrations

Here is the grand test: are the definite and indefinite integrations equivalent? First, evaluate the indefinite integral from ν_1 to ν_2.

$\mathrm{subs}(x = \nu_2, \mathrm{rhs}(indef)) - \mathrm{subs}(x = \nu_1, \mathrm{rhs}(indef))$

$\mathrm{cost}(\%)$

$$595\ additions + 1528\ multiplications + 160\ divisions + 52\ functions + 722\ subscripts$$

Subtract the definite integration from this and simplify the horrible result.

$\mathrm{expand}(\%\% - \mathrm{rhs}(defint))$

$\mathrm{cost}(\%)$

$$8687\ additions + 48796\ multiplications + 3120\ divisions + 8816\ functions + 13360\ subscripts$$

$\mathrm{collect}(\%\%, [\sin, \cos, \mathrm{seq}(a_k, k = 0 .. 4), \nu_1, \nu_2], factor)$

$$0$$

Whew!! That was worth the wait.

A Real-Life Example (continued)

- Finally, after an immense amount of simplification, the answer:

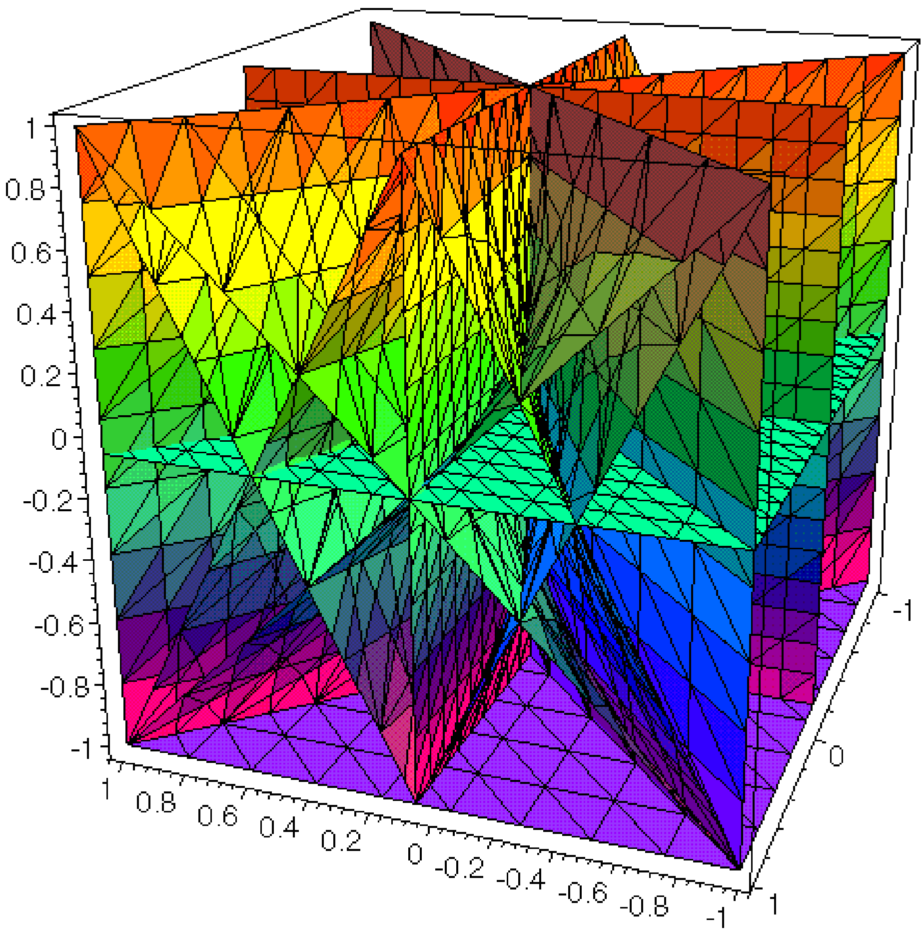
$$S(r,s,g,T,v_1,v_2)=I(v_2)-I(v_1)$$

where

$$
\begin{aligned}
I(x)= & \left\{\frac{a_0+a_1x+a_3x^3+a_2x^2+a_4x^4}{4[2s+r(1-g)]}-\frac{a_2+3a_3x+6a_4x^2}{2[2s+r(1-g)]^3}+\frac{6a_4}{[2s+r(1-g)]^5}\right\}\sin\langle[2s+r(1-g)]x\rangle \\
&+\left\{\frac{a_0+a_1x+a_3x^3+a_2x^2+a_4x^4}{4[2s-r(1-g)]}-\frac{a_2+3a_3x+6a_4x^2}{2[2s-r(1-g)]^3}+\frac{6a_4}{[2s-r(1-g)]^5}\right\}\sin\langle[2s-r(1-g)]x\rangle \\
&-\left\{\frac{a_0+a_1x+a_2x^2+a_3x^3+a_4x^4}{4[2s+r(1+g)]}-\frac{a_2+3a_3x+6a_4x^2}{2[2s+r(1+g)]^3}+\frac{6a_4}{[2s+r(1+g)]^5}\right\}\sin\langle[2s+r(1+g)]x\rangle \\
&-\left\{\frac{a_0+a_1x+a_2x^2+a_3x^3+a_4x^4}{4[2s-r(1+g)]}-\frac{a_2+3a_3x+6a_4x^2}{2[2s-r(1+g)]^3}+\frac{6a_4}{[2s-r(1+g)]^5}\right\}\sin\langle[2s-r(1+g)]x\rangle \\
&+\left\{\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{4[2s+r(1-g)]^2}-\frac{3a_3+12a_4x}{2[2s+r(1-g)]^4}\right\}\cos\langle[2s+r(1-g)]x\rangle \\
&+\left\{\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{4[2s-r(1-g)]^2}-\frac{3a_3+12a_4x}{2[2s-r(1-g)]^4}\right\}\cos\langle[2s-r(1-g)]x\rangle \\
&-\left\{\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{4[2s+r(1+g)]^2}-\frac{3a_3+12a_4x}{2[2s+r(1+g)]^4}\right\}\cos\langle[2s+r(1+g)]x\rangle \\
&-\left\{\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{4[2s-r(1+g)]^2}-\frac{3a_3+12a_4x}{2[2s-r(1+g)]^4}\right\}\cos\langle[2s-r(1+g)]x\rangle \\
&+\left[\frac{a_0+a_1x+a_3x^3+a_2x^2+a_4x^4}{16(s+rg)}-\frac{a_2+3a_3x+6a_4x^2}{32(s+rg)^3}+\frac{3a_4}{32(s+rg)^5}\right]\sin[2(s+rg)x] \\
&+\left[\frac{a_0+a_1x+a_3x^3+a_2x^2+a_4x^4}{16(s-rg)}-\frac{a_2+3a_3x+6a_4x^2}{32(s-rg)^3}+\frac{3a_4}{32(s-rg)^5}\right]\sin[2(s-rg)x] \\
&+\left[\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{32(s+rg)^2}-\frac{3a_3+12a_4x}{64(s+rg)^4}\right]\cos[2(s+rg)x] \\
&+\left[\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{32(s-rg)^2}-\frac{3a_3+12a_4x}{64(s-rg)^4}\right]\cos[2(s-rg)x] \\
&+\left[\frac{a_0+a_1x+a_3x^3+a_2x^2+a_4x^4}{16(s+r)}-\frac{a_2+3a_3x+6a_4x^2}{32(s+r)^3}+\frac{3a_4}{32(s+r)^5}\right]\sin[2(s+r)x] \\
&+\left[\frac{a_0+a_1x+a_3x^3+a_2x^2+a_4x^4}{16(s-r)}-\frac{a_2+3a_3x+6a_4x^2}{32(s-r)^3}+\frac{3a_4}{32(s-r)^5}\right]\sin[2(s-r)x] \\
&+\left[\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{32(s+r)^2}-\frac{3a_3+12xa_4}{64(s+r)^4}\right]\cos[2(s+r)x] \\
&+\left[\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{32(s-r)^2}-\frac{3a_3+12xa_4}{64(s-r)^4}\right]\cos[2(s-r)x] \\
&+\left[\frac{a_0+a_1x+a_2x^2+a_3x^3+a_4x^4}{2r(1+g)}-\frac{a_2+3a_3x+6a_4x^2}{(1+g)^3r^3}+\frac{12a_4}{(1+g)^5r^5}\right]\sin[r(1+g)x] \\
&-\left[\frac{a_0+a_1x+a_2x^2+a_3x^3+a_4x^4}{2r(1-g)}-\frac{a_2+3a_3x+6a_4x^2}{(1-g)^3r^3}+\frac{12a_4}{(1-g)^5r^5}\right]\sin[r(1-g)x] \\
&+\left[\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{2(1+g)^2r^2}-\frac{3a_3+12a_4x}{(1+g)^4r^4}\right]\cos[r(1+g)x] \\
&-\left[\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{2(1-g)^2r^2}-\frac{3a_3+12a_4x}{(1-g)^4r^4}\right]\cos[r(1-g)x] \\
&-\left(\frac{a_0+a_1x+a_2x^2+a_3x^3+a_4x^4}{8rg}-\frac{a_2+3a_3x+6a_4x^2}{16g^3r^3}+\frac{3a_4}{16g^5r^5}\right)\sin(2rgx) \\
&-\left(\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{16g^2r^2}-\frac{3a_3+12a_4x}{32g^4r^4}\right)\cos(2rgx) \\
&-\left(\frac{a_0+a_1x+a_3x^3+a_2x^2+a_4x^4}{4s}-\frac{a_2+3a_3x+6a_4x^2}{8s^3}+\frac{3a_4}{8s^5}\right)\sin(2sx) \\
&-\left(\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{8s^2}-\frac{3a_3+12a_4x}{16s^4}\right)\cos(2sx) \\
&-\left(\frac{a_0+a_1x+a_3x^3+a_2x^2+a_4x^4}{8r}-\frac{a_2+3a_3x+6a_4x^2}{16r^3}+\frac{3a_4}{16r^5}\right)\sin(2rx) \\
&-\left(\frac{a_1+2a_2x+3a_3x^2+4a_4x^3}{16r^2}-\frac{3a_3+12a_4x}{32r^4}\right)\cos(2rx) \\
&+\frac{1}{120}x(60a_0+30a_1x+20a_2x^2+15a_3x^3+12a_4x^4)
\end{aligned}
$$

A Real-Life Example (continued)

- However, we find a problem: singularity surfaces in the parameter space (r,s,g).



In Conclusion

- Computer algebra, when used properly, can be an extremely useful and versatile tool.
  - throw around terrifyingly large expressions without breaking a sweat (or sharpening pencils)
  - make use of all the mathematics you know (and even some you don't know)
    - geometry, algebra, calculus, topology, differential equations, etc.
  - perfect for exploring ideas and persuing hunches
- Can it replace pencil and paper? YES!
- Can it do any of your thinking for you, even just a little bit? NO!
  - In fact, you have to be just as careful, and think even harder, than before.
- If Physics is the art of approximation, then Computer Algebra is the art of squeezing unwieldy expressions.
- See http://aa.usno.navy.mil/Murison/Maple/ for examples.