Integration in terms of exponential integrals and incomplete gamma functions

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Introduction

What is FriCAS?

- FriCAS is an advanced computer algebra system
- forked from Axiom in 2007
- about 30% of mathematical code is new compared to Axiom
- about 200000 lines of mathematical code
- math code written in Spad (high level strongly typed language very similar to FriCAS interactive language)
- runtime system currently based on Lisp

Some functionality added to FriCAS after fork:

- several improvements to integrator
- limits via Gruntz algorithm
- knows about most classical special functions
- guessing package
- package for computations in quantum probability
- noncommutative Groebner bases
- asymptotically fast arbitrary precision computation of elliptic functions and elliptic integrals
- new user interfaces (Emacs mode and Texmacs interface)

FriCAS inherited from Axiom good (probably the best at that time) implementation of Risch algorithm (Bronstein, ...)

- strong for elementary integration
- when integral needed special functions used pattern matching

Part of motivation for current work came from Rubi testsuite: Rubi showed that there is a lot of functions which are integrable in terms of relatively few special functions.

- Adapting Rubi looked difficult
- Previous work on adding special functions to Risch integrator was widely considered impractical

My conclusion:

Need new algorithmic approach. Ex post I claim that for considered here class of functions extension to Risch algorithm is much more powerful than pattern matching.

Informally

$$Ei(u)' = u' \exp(u)/u$$

$$\Gamma(a, u)' = u' u^{m/k} \exp(-u)$$

for $a = (m + k)/k$ and $-k < m < 0$.
Our extension is very natural:

$$\log(x - x_0)' = \frac{1}{x - x_0}$$

$$\mathrm{Ei}(x - x_0)' = \frac{\exp(x - x_0)}{x - x_0}$$

Exponential integral plays the same role for integrals containing exponential function as logarithm plays for rational functions!
Incomplete Gamma functions is has related role: it allows integrating functions of form $x^{k+m-1} \exp(x^k)$.

Simple examples

```
integrate(exp(x)/x^2, x)
```

$$\frac{-e^x + x\ Ei\left(x\right)}{x}$$

Needs preprocessing (Hermite reduction) to see Ei term.

```
integrate((x-1)*exp(x)/x^2, x)
```

$$\frac{e^x}{x}$$

Similar looking, but elementary.

```
integrate(exp(x)/(x^2 - 2), x)
```

$$\frac{Ei\left(-\sqrt{2}+x\right)\left(e^{\sqrt{2}}\right)^{2} - Ei\left(\sqrt{2}+x\right)}{2\sqrt{2}\,e^{\sqrt{2}}}$$

Single exponential and denominator irreducible over integers, but two Ei terms.

```
x*exp(x^2)/(x^4-5)
```

$$\frac{\sqrt{5}\,Ei\left(-\sqrt{5}+x^{2}\right)\left(e^{\sqrt{5}}\right)^{2} - \sqrt{5}\,Ei\left(\sqrt{5}+x^{2}\right)}{20\,e^{\sqrt{5}}}$$

Similar, but relation between complex factors of denominator and Ei terms is more complicated.

```
integrate(((x+1)*exp(x))/log(x*exp(x)), x)
```

$$li\left(x\,e^{x}\right)$$

This shows that result may appear as logarithmic integral.

```
integrate(((x+1)*exp(x))/(x + log(x)), x)
```

$$li\left(x\,e^{x}\right)$$

This shows that system can perform necessary simplifications.

```
integrate(exp(-x^2+2*x), x)
```

$$\frac{e\,\mathrm{erf}\left(x-1\right)\,\sqrt{\pi}}{2}$$

```
D(%, x)
```

$$e\,\,e^{-x^2+2\,\,x-1}$$

erf term with a shift.

```
integrate((2*x+4)*exp(-x^2-2*x-1)/(x+1), x)
```

$$\mathrm{erf}\left(x+1\right)\,\sqrt{\pi}+Ei\left(-x^2-2\,\,x-1\right)$$

This shows that Ei and erf may be mixed together.

```
integrate((1 + exp(x))*exp(exp(x)^2), x)
```

$$\frac{\sqrt{\pi}\ \mathit{erfi}\left(e^{x}\right)+\mathit{Ei}\left(e^{x\,2}\right)}{2}$$

Similar, but no denominator to signal presence of Ei term. Also, we get erfi when appropriate.

```
integrate(x^3*exp(-x^3), x)
```

$$\frac{-\Gamma\left(\frac{1}{3},\ x^{3}\right)-3\ x\ e^{-x^{3}}}{9}$$

Gamma plus elementary part.

```
integrate((x+1)*exp(-x^3-3*x^2-3*x), x)
```

$$-\frac{e\ \Gamma\left(\frac{2}{3},\ x^{3}+3\ x^{2}+3\ x+1\right)}{3}$$

Gamma with a shift.

```
integrate(x^2*exp(-(x+1)^3), x)
```

$$\frac{2\,\Gamma\left(\frac{2}{3},\, x^3+3\,x^2+3\,x+1\right)-\Gamma\left(\frac{1}{3},\, x^3+3\,x^2+3\,x+1\right)-e^{-x^3-3\,x^2-3}}{3}$$

Single term in the input, two Gamma terms plus elementary part in the output.

```
integrate(sin(x+1)/x^2, x)
```

$$\frac{-2\,\sin(x+1)-2\,x\,\sin(1)\,\mathit{Si}(x)+x\,\cos(1)\,\mathit{Ci}(x)+x\,\cos(1)\,\mathit{Ci}(-x)}{2\,x}$$

Si and Ci terms with shift.

```
integrate(x*sin(x^4), x)
```

$$\frac{\mathit{fresnelS}\left(x^2\,\sqrt{\frac{2}{\pi}}\right)}{2\,\sqrt{\frac{2}{\pi}}}$$

can generate Fresnel integrals.

```
integrate(exp(x + sqrt(x+1)), x)
```

$$\frac{2\ e^{\frac{5}{4}}\ e^{\sqrt{x+1}+x} - \sqrt{\pi}\ \mathit{erfi}\left(\frac{2\ \sqrt{x+1}+1}{2}\right)}{2\ e^{\frac{5}{4}}}$$

we can handle some algebraics by cheating (change of variable).

```
f := (2*x^4-x^3+3*x^2+2*x+2)*exp(x/(x^2+2))/(x^3+2*x)
integrate(f, x)
```

$$\left(x^2+2\right)\ e^{\frac{x}{x^2+2}} + \mathrm{Ei}\left(\frac{x}{x^2+2}\right)$$

Hard to separate elementary and Ei part.

Peek inside

```
)trace INTEF )math
integrate(sin(x^2), x)

 1<enter ElementaryIntegration.lfintegrate,43 :
                  2 2
              %i x
      - %i (%e      )  + %i
 arg1= --------------------
                   2
               %i x
            2%e
 arg2= x
 1>exit  ElementaryIntegration.lfintegrate,43 :
           +---+
           | 2
 fresnelS(x |--- )
          \|%pi
 -----------------
```

Theoretical background

If K is a differential field, $v, u \in K$ and $v' = u'/u$ we say that u is exponential element and that v is logarithmic element. The set of exponential elements in K is an abelian group with respect to multiplication. The set of logarithmic elements in K is an abelian group with respect to addition.
Main examples:

- explicit exponential is exponential element
- argument of logarithm is exponential element
- if a^k is an exponential element, then a is also an exponential element

Example: If $K = F(\theta)$, θ is Lambert W over F, that is θ is transcendental and there exist $z \in F$ such that $\theta' = \frac{z'\theta}{z(\theta+1)}$, then θ/z is an exponential element in K and $-\theta$ is corresponding logarithmic element.

Theorem

If K is finitely generated differential field, then group of logarithmic elements modulo additive constants is a finite rank free abelian group. The same for group of exponential elements modulo multiplicative constants.

In our fields we can effectively test if element is an exponential element and find associated logarithmic element and vice versa.

Gamma extensions

We say that a differential field E is a gamma extension of F if there exists $\theta_1, \ldots, \theta_n \in E$ such that $E = F(\theta_1, \ldots, \theta_n)$ and for each i, $1 \leq i \leq n$, one of the following holds

1. θ_i is algebraic over F_i
2. $\frac{\theta_i'}{\theta_i} = u'$ for some $u \in F_i$
3. $\theta_i' = \frac{u'}{u}$ for some $u \in F_i$
4. $\theta_i' = \frac{u'}{v}$ for some $u, v \in F_i$ such that $u' = v'u$
5. there are $w, u, v \in F_i$ and integers k, m such that $\theta_i' = wu'$, $u' = v'u$, $w^k = v^m$, $-k < m < 0$.

where $F_i = F(\theta_1, \ldots, \theta_{i-i})$.

Liouville principle

Let $f \in K(\theta)$ where θ is a exponential or a primitive. Under appropriate technical assumptions, if f has integral in a Gamma extension of $K(\theta)$, then there is an algebraic extension $\bar{K}$ of K such that

$$f = v_0' + \sum_{i \in I_1} c_i \frac{v_i'}{v_i} + \sum_{i \in I_2} c_i v_i' \frac{u_i}{v_i} + \sum_{i \in I_3} c_i v_i' w_i u_i \qquad (1)$$

where $c_i \in K$ are constants, $u_i' = v_i' u_i$, $v_i \in K(\theta)$ for $i \in I_2 \cup I_3$, $u_i \in K(\theta)$ for $i \in I_2$, $u_i, w_i \in \bar{K}(\theta)$, $w_i u_i \in K(\theta)$ for $i \in I_3$, $w_i^{k_i} = v_i^{m_i}$.

The main case is integration of functions of form $f\theta$ where θ is an exponential. We get equation:

$$f\theta = (g\theta)' + \sum_{i \in I_2} v_i' \frac{u_i \theta}{v_i} + \sum_{i \in I_3} v_i' w_i u_i \theta$$

where $v_i' u_i \theta = (u_i \theta)'$.
We will denote logarithm of θ as v, that is $\theta' = v'\theta$. Then we can write

$$f = g' + v'g + \sum_{i \in I_2} v_i' \frac{u_i}{v_i} + \sum_{i \in I_3} v_i' w_i u_i \qquad (2)$$

We will call terms of the sum over I_2 Ei terms and terms of the sum over I_3 gamma terms. Formula 2 generalises Risch differential equation (RDE).

Parametric RDE

Problem: given f_i, u find set of g, c_i such that

$$f_0 = g' + ug + \sum c_i f_i$$

and c_i are constants.
We assume availability of solver for parametric RDE.
In generic case we need to find finite number of candidates for possible Ei and gamma terms and use solver for parametric RDE.
In few special cases we have infinite number of candidate Ei or gamma terms and determine which terms actually occur during solving RDE.

The following cases may appear:

- regular Ei terms, depend only on denominator of f
- special Ei terms, depend only on structure of differential field
- infinite family of Ei terms in case of v linear in logarithm
- regular gamma terms, depend only on structure of differential field
- infinite families of gamma (erf) terms

General setup

Let ψ be top transcendental in K and M be a differential subfield such that K is algebraic over $M(\psi)$. By assumption we can write $v_i = v + r_i\psi + a_i$ where $a_i \in M$ and $r_i \in \mathbb{Q} \neq 0$ only when ψ is a logarithm.
When ψ is not an exponential let S be integral closure of $M[\psi]$ in K. When ψ is an exponential let S be integral closure of $M[\psi, \psi^{-1}]$. (In general we put inverses of all special elements in S). We can write elements of f as quotient with numerator in S and denominator in $M[\psi]$. When ψ is an exponential we additionally may assume that denominator is relatively prime to ψ.

Notation:

$$v_{r,a} = v + r\psi + a$$

$N_{r,a}$ is norm of numerator of $v_{r,a}$.
L_r is norm of numerator of $\partial_\psi v_{r,a}$.
P is norm of numerator of $\partial_\psi^2 v$.

Ei terms

Theorem

If $v_i' \frac{u_i}{v_i}$ is an Ei term appearing in formula 2 and p is a prime divisor such that $\mathrm{ord}_p(v_i) > 0$. Then $\mathrm{ord}_p(E) > 0$.

Corollary: $\mathrm{Res}(N_{r,a}, E) = 0$.
Problem: If ψ is a logarithm we need more equations.
Solution: If denominator of v is divisible by two prime divisors we combine constraints from both divisors.
In transcendental case we just can use $\mathrm{Res}(N_{r,a}, E) = 0$ and $\partial_\psi \mathrm{Res}(N_{r,a}, E) = 0$.

Ei cases

Algebraic constants

$$\exp(x)/(x^2-5) = e^{\sqrt{5}}\mathrm{Ei}(x-\sqrt{5})' - e^{-\sqrt{5}}\mathrm{Ei}(x+\sqrt{5})'$$

In general, if p is irreducible polynomial with constant coefficients, c_i are roots of p, d_i are nonzero constants and $\mathrm{Ei}(\phi)'$ has denominator D, then $\sum d_i \mathrm{Ei}(\phi + c_i)'$ has denominator $\prod(D + c_i)$.
In our method we get polynomial equation $q(a) = 0$ for possible shifts. Each irreducible factor q_i of q corresponds to orbit of single logarithmic element by algebraic shifts. The second highest coefficient of q_i gives trace $\tilde{a}$ of a. Shifting arguments of q_i by $-\tilde{a}$ we get equation for algebraic shifts.

Factors in higher powers

$$x \exp(\log(x)^2)/(\log(x)+1) = \mathrm{Ei}((\log(x)+1)^2)'/(2e)$$

extra equation comes from condition that $v_{r,a}$ is divisible by a square.

Overlapped factors

$$\frac{(x^2(2\log(x)^2+3\log(x))+(2\log(x)^2+5\log(x)+2))\exp(\log(x)^2)}{\log(x)(\log(x)+1)(\log(x)+2)} =$$

$$(\mathrm{Ei}((\log(x)+1)(\log(x)+2))'/e^2 + \mathrm{Ei}(\log(x)(\log(x)+1))'.$$

Actually, no problem for our method but may confuse systems using partial fraction decomposition.

Special terms

$$\exp(\exp(x)/(\exp(x)+1)) = \mathrm{Ei}\left(\frac{e^x}{e^x+1}\right)' - e\mathrm{Ei}\left(-\frac{1}{e^x+1}\right)'$$

When ψ is an exponential than we check if $v + a$ can reduce to a monomial.

$$\exp(x - \log(x)) = Ei(x)'$$

When ψ is a logarithm degree at infinity can drop to 0. In transcendental case this can only happen if v is a polynomial of degree 1 in ψ with integer leading coefficient. In such case we can reduce integral to integral with $v \in M$. In algebraic case there are finitely many values of r which may lead to zeros at infinity, we need to handle them separately.

Infinite family

$$\mathrm{Ei}((c+k)\log(x))' = \frac{\exp((c+k)\log(x))}{x\log(x)} = \frac{x^{k-1}\exp(c\log(x))}{\log(x)}$$

so we get infinite family of Ei terms with the same denominator. Can happen only if v is linear in ψ. We can reduce the problem to $f \in M$ and then to equation

$$\tilde{f} = \sum c_k z^k$$

with constant c_k.

Completing powers

To find Gamma terms we search for r, v such that $v_{r,a}$ is a power modulo multiplication by exponentials. Main idea is that exponentials have no nontrivial divisors, so that if $v_{r,a}$ is divisible by a nontrivial divisor p and $v_{r,a}$ is a k-th power, then k is divisible by p^k. To test for divisibility by power of divisors we use GCD with derivative. More precisely, if $v_{r,a}$ is divisible by p^2 than $N_{r,a}$ and L_r have common factor, that is $\mathrm{Res}(N_{r,a}, L_r) = 0$. This works if ψ is not a logarithm. For $k \geq 3$ we get second equation using second derivative. For $k = 2$ (that is erf terms) we need to check for presence of two zeros of multiplicity 2. In case of single zero of multiplicity 2 there is possibility for infinite family ("movable zero").

$$\exp(-x^2 - \mathrm{erf}(x)^2)$$

$\psi = \mathrm{erf}(x)$, $v_a = -\psi^2 - x^2 + a$, $\partial_\psi v_a = -2\psi$, $\mathrm{Res}(v_a, \partial_\psi v_a) = 4(a - x^2)$, $\mathrm{Res}(v_a, \partial_\psi v_a) = 0$ iff $a = x^2$, so $v_a = -\psi^2$ and the corresponding term is $\mathrm{erf}(\mathrm{erf}(x))'$.

It may happen that there are no nontrivial zeros:

$$f = \Gamma(1/3, \exp(x))' = \exp(-\exp(x) + x/3).$$

We have $u_1 = \exp(-\exp(x))$, $v_1 = -\exp(x)$ and $w_1 = \exp(x/3)$.
Variation: $f = \mathrm{erf}(\exp(3x/2))' = \exp(-\exp(x)^3 + 3x/2)$.
The a term is uniquely determined by condition that $v + a$ contains only one term. Consequently the gamma term is uniquely determined and can appear only if v is a monomial or a binomial.

$$\sqrt{\pi}\mathrm{erf}(\sqrt{x})' = \exp(-x)/\sqrt{x} = \exp(-x - \log(x)/2)$$

Non reduced case.

Movable zeros

There are four cases where we get infinite families divisible by a square of prime divisor:

- $v = b\psi^2 + c\psi + d$ is quadratic polynomial
- $v = b\psi + c + dy$ where $y^2 = \sqrt{e\psi + f}$
- $v = b\psi + c + dy$ where $y^2 = \sqrt{e\psi^2 + f\psi + g}$
- $$v = \frac{b\psi^2 + c\psi + d}{\psi + e}$$

In integration context there are extra constraints and they eliminate the second family. For the three other families we show via examples that they may appear during integration.

Infinite families

$$\sqrt{\pi}\mathrm{erf}(\log(x)+k)' = 2x^{-1}\exp(-\log(x)^2 - 2k\log(x) - k^2)$$
$$= 2\exp(-k^2)x^{2k-1}\exp(-\log(x)^2).$$

This one is due to Cherry and he also gave method to handle it.

$$\sqrt{\pi}\mathrm{erfi}\left(\frac{k\log(\log(x))+\log(x)/2}{\sqrt{\log(\log(x))}}\right)' =$$

$$\frac{2(\log(x)+k)\log(\log(x))-\log(x)}{2x\log(x)\log(\log(x))\sqrt{\log(\log(x))}}\times$$

$$\exp\left(\frac{4k^2\log(\log(x))^2+4k\log(x)\log(\log(x))+\log(x)^2}{4\log(\log(x))}\right) =$$

$$((\log(x)+k)\log(\log(x))-\log(x)/2)\log(x)^{k^2-1}x^{k-1}\times$$

$$\exp\left(\frac{\log(x)^2}{4\log(\log(x))}-3\log(\log(\log(x)))/2\right)$$

In general can happen when ψ is a logarithm and $v = (b\psi^2 + c\psi + d)/\psi - 3/2\log(\psi)$. Then b is a constant. We can reduce problem to

$$A\psi + B = \sum_{I_3} v_i' w_i u_i.$$

This is the most complicated case. We get a quadratic relation between a and r. Depending on this relation we have further subcases:

- change of variables reduces problem to different case
- a is uniquely determined by r. Can use method similar to quadratic case
- a is a constant. Need to solve $C = \sum d_r z^r$ where d_r are unknown constants and z and C are known
- can use one coordinate of a to parametrise solutions. Need to solve $C = \sum d_k z_1^r z_2^k$ where d_r are unknown constants, z_1 and z_2 are known and r is quadratic function of k.

The last subcase is most tricky to solve. We use a single pole of z_1 to get bound on k. More precisely, the problem is that there may be two values of k_1, k_2 such that $z_1^r(k_i)z_2^{k_i}$ have pole of the same maximal order and the constants are such that

$$d_{k_1} z_1^r(k_1) z_2^{k_1} + d_{k_2} z_1^r(k_2) z_2^{k_2}$$

is of lower order. However we can look at highest order term in such combination — difference between order of linear combination and order of terms is bounded by a constant. Since orders of terms grow quadratically there is gap between orders of consecutive terms growing linearly in $|k|$. So for $|k|$ large enough the can be no cancellation between highest order term of linear combination above and lower order terms.
Examples were known, but there were no theory how to handle them.

If $y = \sqrt{\log(x)^2 - 1}$, $\phi = \log(x) + y$, $v = y$, $\gamma = \sqrt{k^2 - 1}/k$, then

$$\sqrt{\pi}\mathrm{erfi}(\frac{k(\phi+\gamma)}{\sqrt{\phi}})' = (k\gamma(\log(x) - 1) - k(\gamma\log(x) - 1)y) \times$$

$$\exp((2k^2 - 1)\log(x) + 2k^2\gamma + y)/\sqrt{\phi} =$$

$$(k\gamma(\log(x) - 1) - k(\gamma\log(x) - 1)y)\, x^{2k^2-1} \times$$

$$\exp(2k^2\gamma)\exp(y + \log(\phi)/2)$$

so we get infinite family of erf terms. The example above contains new constants γ and $\exp(2k^2\gamma)$. $\exp(2k^2\gamma)$ is a multiplicative factor so we can simply omit it. γ plays nontrivial role but taking trace with respect to γ we get example with rational coefficients:

$$k(-1 + y)x^{2k^2-1}\exp(y + \log(\phi)/2).$$

In general we have $v = b\phi + c + dy + \log(\phi)/2$ with $y^2 = e\psi^2 + f\psi + g$, $\phi = h(\psi + ty)$, $et^2 = 1$, $h \in M$. Method of solving is similar to previous examples. In particular, infinite family is possible only when b, d^2e and $(f^2 - 4eg)/e^2$ are constants and we have linear relation between r and a'.

Thank you