Loop integral computation in the Euclidean or physical kinematical region using numerical integration and extrapolation

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Introduction - Overview

– Accurate theoretical predictions are needed in view of improvements in the technology of high energy physics experiments.

– Higher order corrections are required for accurate theoretical predictions of the cross-section for particle interactions.

– The Feynman diagrammatic approach is commonly used to address higher order corrections, and Feynman loop integrals arise in the calculations.

– Loop integrals may suffer from integrand singularities or irregularities at the boundaries and/or in the interior of the integration domain (for physical kinematics).

– We implemented iterated integration numerically using one- or low-dimensional adaptive integration algorithms in subsequent coordinate directions, enabling intensive subdivision in the vicinity of singularities.

Introduction - Overview

– To handle a singularity in the domain interior, we add a term $(-i\varrho)$ in the denominator, and perform a nonlinear extrapolation (as $\varrho \to 0$) to a sequence of integrals obtained for a (geometrically) decreasing sequence of ϱ.

– UV singularities are treated by dimensional regularization, where the space-time dimension $\nu = 4$ is replaced by $\nu = 4 - 2\varepsilon$ for a sequence of ε values, and a linear extrapolation is applied as $\varepsilon \to 0$.

– Presence of both types of singularities warrants a double extrapolation.

– The code is further multi-threaded to run in a shared memory environment. We will demonstrate the combined methods for sample diagrams.

Loop integral - Representation

L-loop integral with N internal lines

$$\mathcal{I} = \Gamma(N - \frac{\nu L}{2})\,(-1)^N \int_{\mathcal{C}_N} \prod_{r=1}^{N} dx_r\, \delta(1 - \sum x_r)\, U^{-\nu/2} (V - i\varrho)^{\nu L/2 - N}$$

$$= \Gamma(N - \frac{\nu L}{2})\,(-1)^N \int_{\mathcal{S}_{N-1}} \prod_{r=1}^{N-1} dx_r\, U^{-\nu/2} (V - i\varrho)^{\nu L/2 - N}$$

where $V = M^2 - W/U$, $M^2 = \sum_r m_r^2 x_r$;
U and W are polynomials determined by the topology of the corresponding diagram and physical parameters; $\nu = 4 - 2\varepsilon$ is the space-time dimension;

$\mathcal{C}_N =$ the N-dimensional unit hypercube; $\mathcal{S}_d = \{\mathbf{x} \in \mathcal{C}_d \mid \sum_{j=1}^{d} x_j \leq 1\}$ is the d-dimensional unit simplex.

Asymptotics

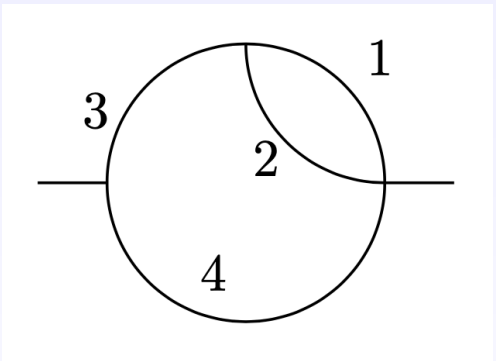
Asymptotic expansion (as $\varepsilon \to 0$)

$$\mathcal{I} = \mathcal{I}(\varepsilon) \sim \sum_{k \geq \kappa} C_k \, \varepsilon^k$$

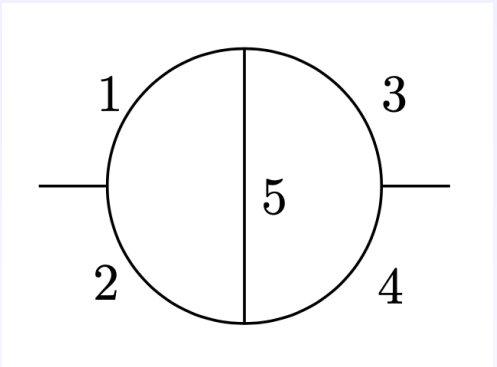
$\kappa = -2$ for the cases considered.

$\mathcal{I}(\varepsilon) \sim C_{-2}/\varepsilon^2 + C_{-1}/\varepsilon + C_0 + \ldots$

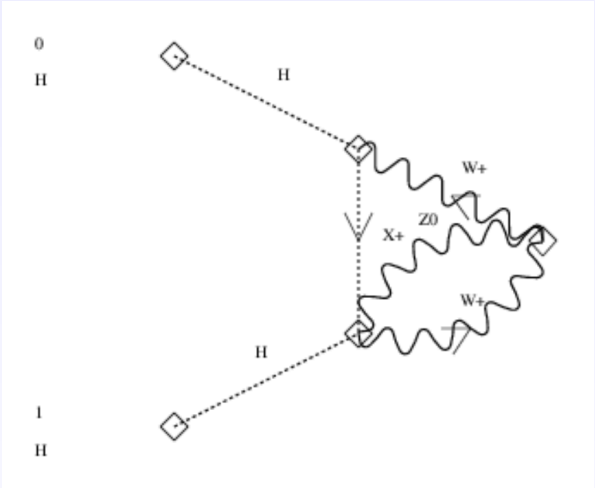
Sample diagrams



(a)



(b)



(c)

Figure: Sample diagrams (a) Lemon, $N = 4$; (b) Magdeburg, $N = 5$; (c) Graph 2116, $N = 4$ [7]

Specifications [9]

Lemon, Graph 2116

$U = x_{12}x_{34} + x_1x_2, \quad W = s\,(x_4(x_1x_2 + x_1x_3 + x_2x_3))$
$x_{k\ell\ldots n} = x_k + x_\ell + \ldots + x_n$
Cases:
$m_1 = m_2 = m_3 = m_4 = 1$ (lemon1111)
Graph 2116 (Z, W, W, χ): In units of $M_H = 1$, $M_W = 0.64308$ and $M_Z = 0.7295008$, $M_\chi = M_W$.

Magdeburg

$U = x_{12}x_{34} + x_{1234}x_5, \quad W = s\,(x_1x_2x_{34} + x_3x_4x_{12} + x_{13}x_{24}x_5)$

Case: $m_1 = m_2 = m_3 = m_4 = m_5 = 1$

Methods: Automatic Integration

Black-box approach to produce (as outputs) an approximation $Q(f)$ to an integral

$$If = \int_{\mathcal{D}} f(\vec{x})\, d\vec{x}$$

and an error estimate $\mathcal{E}f$ of the actual error $Ef = |Qf - If|$, in order to satisfy an accuracy requirement of the form

$$|\, Qf - If\,| \;\leq\; \mathcal{E}f \;\leq\; \max\{\, t_a\,,\; t_r\,|If|\,\},$$

where the integrand function f, region $\mathcal{D}$ and (absolute/relative) error tolerances t_a and t_r, respectively, are specified as part of the input.

Methods: Automatic Adaptive Integration

Applied in consecutive coordinate directions (using Quadpack DQAGE, and DQAGSE (DQAGE strategy + extrapolation) [11, 3, 5]:

```
Evaluate initial region and update results
Initialize priority queue with initial region
while (evaluation limit not reached and
        estimated error too large)
    Retrieve region from priority queue
    Split region into subregions
    Evaluate new subregions and update results
    Insert new subregions into priority queue
```

Figure: Adaptive Integration Meta-Algorithm

Methods: Iterated Parallel Adaptive Integration

– Integration over a finite d-dimensional product region,

$$\mathcal{I} = \int_{\alpha_1}^{\beta_1} dx_1 \int_{\alpha_2}^{\beta_2} dx_2 \ldots \int_{\alpha_d}^{\beta_d} dx_d \; f\,(x_1, x_2, \ldots, x_d),$$

– The limits of integration may in general be functions, $\alpha_j = \alpha_j(x_1, x_2, \ldots, x_{j-1})$ and $\beta_j = \beta_j(x_1, x_2, \ldots, x_{j-1})$.
– We can integrate over the interval $[\alpha_j, \beta_j]$ with a 1D adaptive integration code.
– If an interval $[a, b]$ arises in the subdivision of $[\alpha_j, \beta_j]$ for $1 \leq j < d$, then the local integral approximation over $[a, b]$ is of the form

$$\int_a^b dx_j \; F(c_1, \ldots, c_{j-1}, x_j) \;\approx\; \sum_{k=1}^{K} w_k F(c_1, \ldots, c_{j-1}, x^{(k)}),$$

where w_k and $x^{(k)}$, $1 \leq k \leq K$, are the weights and abscissae of the local rule scaled to the interval $[a, b]$ and applied in the x_j-direction.

Methods: Iterated Parallel Adaptive Integration

– The function evaluation

$$F(c_1, \ldots, c_{j-1}, x^{(k)}) = \int_{\alpha_{j+1}}^{\beta_{j+1}} dx_{j+1} \ldots \int_{\alpha_d}^{\beta_d} dx_d \; f(c_1, \ldots, c_{j-1}, x^{(k)}, x_{j+1}, \ldots, x_d),$$

is itself an integral in the $x_{j+1}, \ldots, x_d$-directions, and is computed by the method(s) for the inner integrations.
– For $j = d$, this is the evaluation of the integrand function

$$F(c_1, \ldots, c_{d-1}, x^{(k)}) = f(c_1, \ldots, c_{d-1}, x^{(k)}).$$

– Subsequently, we give results obtained with 1D iterated integration by the programs DQAGE and DQAGSE from QUADPACK [11, 3], where the local integration is performed with the (7, 15)- or the (10, 21)-points Gauss-Kronrod pairs.

Methods: Iterated Parallel Adaptive Integration

– The inner integrals are independent and can thus be evaluated in parallel, by multiple threads [4] (using, e.g., OpenMP [10]).

– Important properties of this parallelization include:
(1) large granularity of the parallel integration, involving the inner integrations;

(2) apart from possibly the order of the summation in the local rule evaluation, the parallel calculation is the same as the sequential evaluation.

Methods: Double Extrapolation

– Linear extrapolation is based on an asymptotic expansion of the form

$$\mathcal{I}(\varepsilon) \sim \sum_{k \geq \kappa} C_k \, \varphi_k(\varepsilon), \qquad \text{as } \varepsilon \to 0 \tag{1}$$

where the sequence of $\varphi_k(\varepsilon)$ is known.

– Here, $\kappa = -2$ and $\varphi_k(\varepsilon) = \varepsilon^k$.

– The expansion is truncated after $2, 3, \ldots, n$ terms to form linear systems of increasing size in the C_k variables. This is a generalized form of Richardson extrapolation [1, 13].

Methods: Double Extrapolation

– For fixed $\varepsilon = \varepsilon_\ell$, the integral

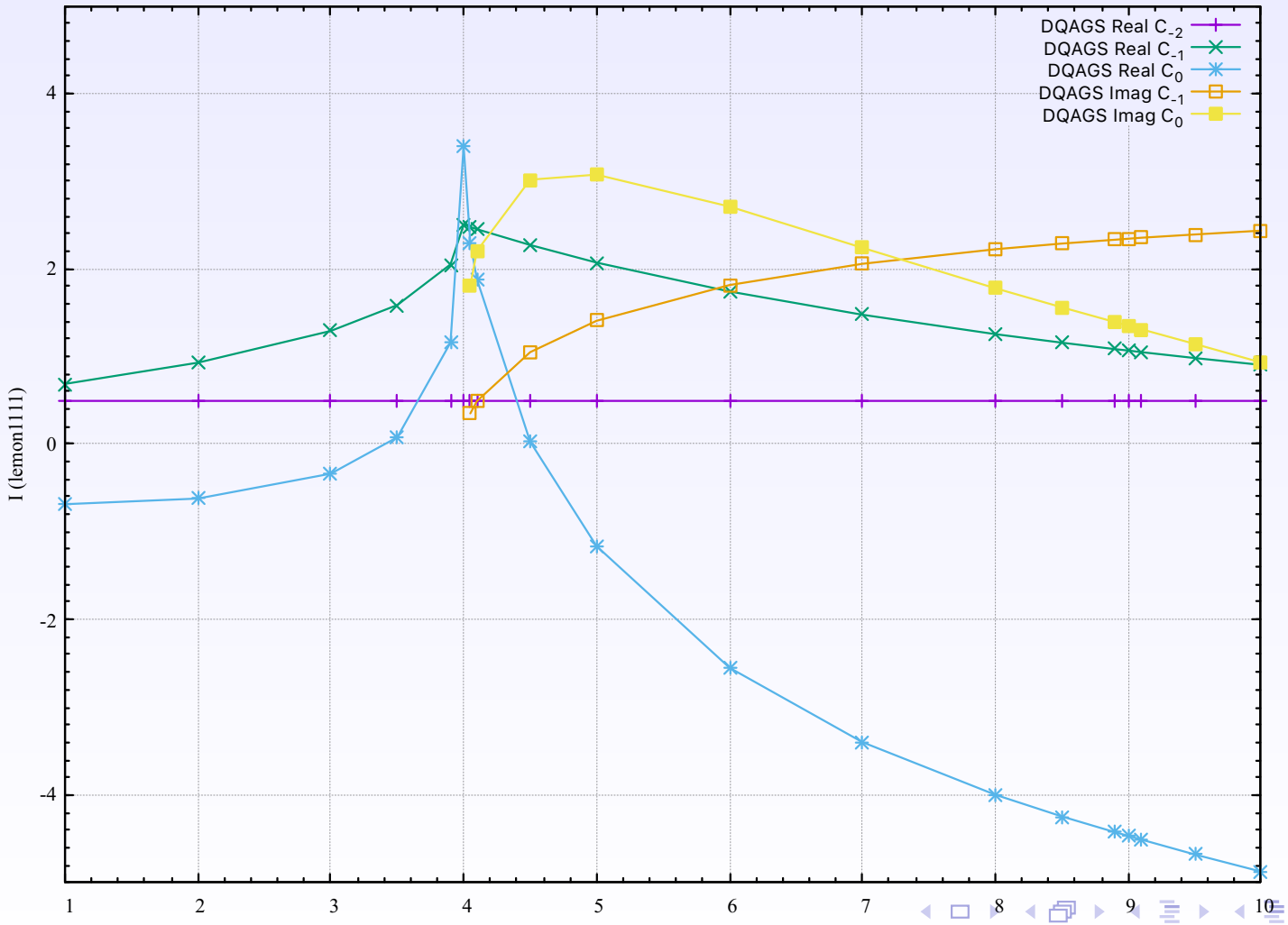
$$\mathcal{I} = \Gamma(N - \frac{\nu L}{2})\,(-1)^N \int_{\mathcal{S}_{N-1}} \prod_{r=1}^{N-1} dx_r\, U^{-\nu/2} (V - i\varrho)^{\nu L/2 - N}$$

may have singularities as $\varrho \to 0$.

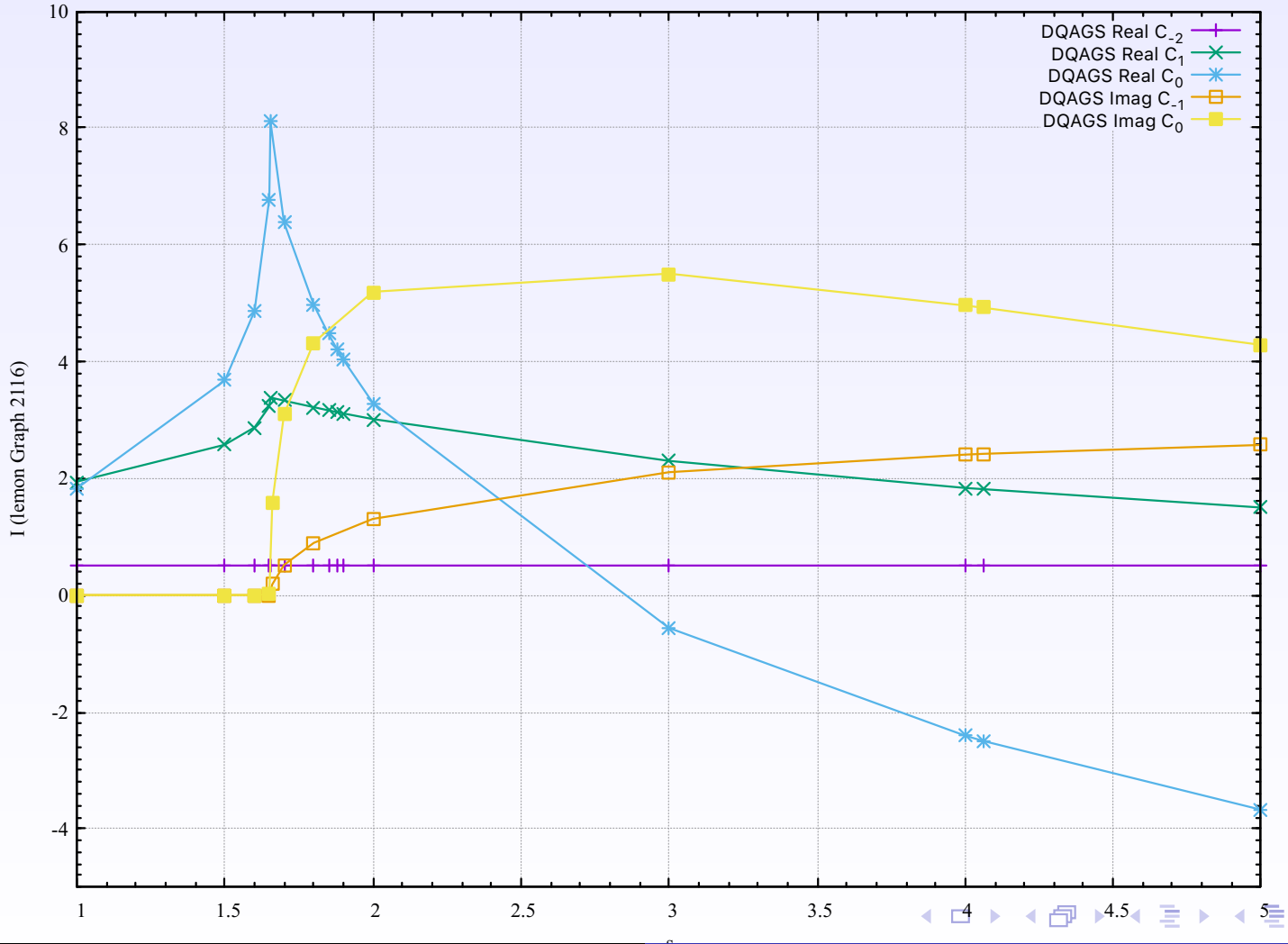
– Since the structure of the expansion in ϱ is unknown, we apply a non-linear extrapolation with the ϵ-algorithm [12, 14] to a sequence of $\mathcal{I}(\varepsilon_\ell, \varrho)$ as $\varrho \to 0$.

– The combined ε and ϱ extrapolations constitute a double extrapolation [2, 6, 15, 8].

Results lemon1111: C_{-2}, C_{-1}, C_0 as a function of s



Results Graph 2116: C_{-2}, C_{-1}, C_0 as a function of s



Results notes

– lemon1111: Pronounced threshold at $s = (1+1)^2 = 4$.
– Threshold at $s = (1+1+1)^2 = 9$ is not pronounced.
– Good comparison with pySecDec results, except for $s = 4$ (where pySecDec returns 0).

– Graph 2116: Pronounced threshold at $s = (2 \times 0.64308)^2 = 1.6542075456$
– Threshold at $s = (2 * 0.64308 + 0.7295008)^2 = 4.06288846065664$ is not pronounced.
– Results were obtained with the particle masses and s in the unit of $M_H^2 = 1$.

– Results for Magdeburg (coefficients) for mass assignments $1111x$ with $x = 0, 1, 2$ were given in [15].

Timing Results DQAGE for Magdeburg as a function of #threads

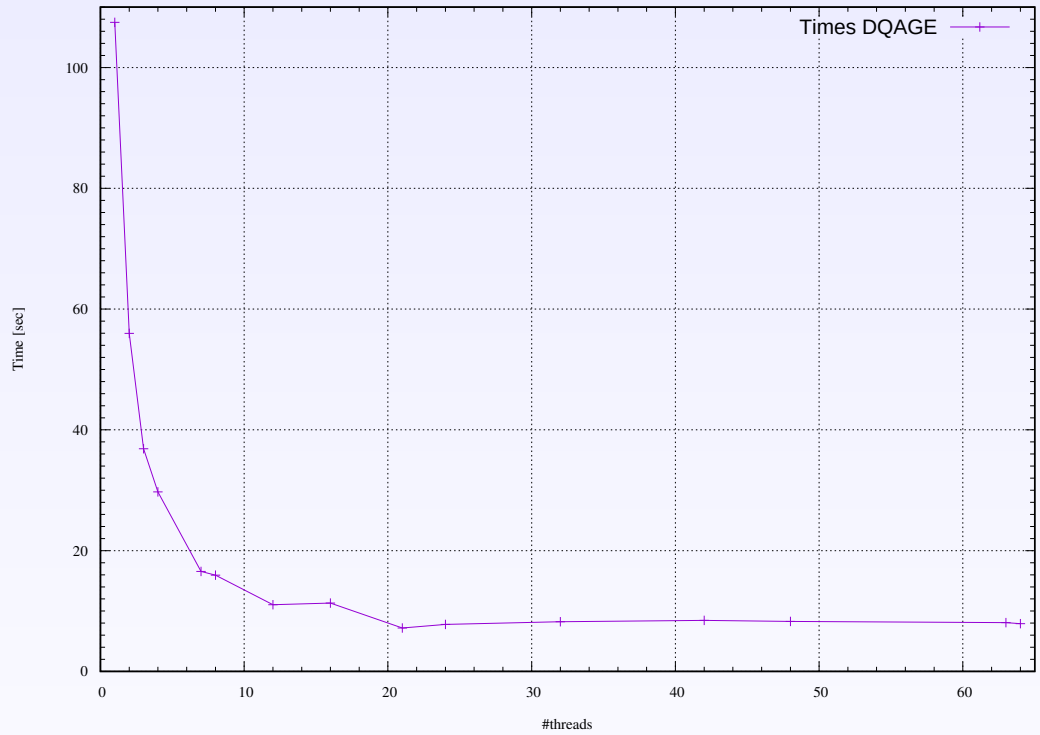


Figure: Magdeburg11111: Parallel times [sec] of DQAGE as a function of #threads, with DQAGE keys 2, 2, 2, 2 (Gauss-Kronrod rule pair with 10-21 points for local integrations), $m_1 = m_2 = m_3 = m_4 = m_5$, $s = 1$, Extrapolation for $\varrho = 2^{-17}, 2^{-18}, \ldots, 2^{-31}$

Conclusions

– Whereas symbolic or symbolic/numerical calculations are performed for some challenging problems using existing software packages, we focus on the development of fully numerical methods for the evaluation of Feynman loop integrals.

– The integration strategies adhere to automatic adaptive integration, which is a black-box approach for generating an approximation, assuming little or no knowledge of the problem, apart from the specification of the integrand function.

– We demonstrated efficient strategies based on iterated integration, multithreading with OpenMP, and double extrapolation.

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