PoisFFT - A Free Parallel Fast Poisson Solver

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Abstract

A fast Poisson solver software package PoisFFT is presented. It is available as a free software licensed under the GNU GPL license. The package uses the fast Fourier transform to directly solve the Poisson equation on a uniform orthogonal grid. It can solve the pseudo-spectral approximation and the second order finite difference approximation of the continuous solution. The paper reviews the mathematical methods for the fast Poisson solver and discusses the software implementation and parallelization. The use of PoisFFT in an incompressible flow solver is also demonstrated.

Keywords: Poisson equation, fast Poisson solver, parallel, MPI, OpenMP

1. Introduction

The Poisson equation is an elliptic partial differential equation with a wide range of applications in physics or engineering. In this paper the form

$$\nabla^2 \varphi = g,$$

(1)

in a rectangular domain $\Omega \subset \mathbb{R}$, for $d = 1 \ldots 3$, with boundary conditions specified on $\partial \Omega$ is considered. The solution $\varphi$ and the specified source term $g$ are both sufficiently smooth real functions on $\Omega$. The equation can be used for computations of electrostatic and gravitational potentials, to solve potential flow of ideal fluids or to perform pressure correction when solving the incompressible Navier-Stokes equations. We assume that $\varphi$ and $g$ are smooth as necessary.

There are many methods for the approximate numerical solution of the Poisson equation. It can be discretized in many ways using the finite difference, finite volume, finite element or (pseudo-)spectral method.

In many problems the goal is to compute the most accurate approximation of the continuous problem, while in other applications it is necessary to use...
the discretization consistent with other parts of a larger solver. This is true in
the incompressible flow solvers where the discrete continuity equation must be
enforced by solving the discrete Poisson equation[1].

The fast direct solvers of the Poisson equation have a long history. The
method of cyclic reduction was used by Hockney [2], Buzbee et al. [3] and
Buneman [4]. The Fourier analysis method was developed by Cooley et al.
[5], Williamson and Ericksen [6] and Swartztrauber [7][8] for various boundary
conditions. The methods of the cyclic reduction and Fourier analysis can
be combined in the FACR algorithm[8]. The discrete Fourier transforms used
with different boundary conditions were surveyed by Schumann and Sweet [9].

The requirement of a rectangular grid or other simple type of grid can be
too restrictive for many applications, but the fast solution on a regular grid can
be often used as a preconditioner for a solution on an unstructured grid or for
problems with non-constant coefficients (e.g., \( \nabla \cdot (a(x) \nabla \phi) = g \))[10].

Many implementations of fast Poisson solvers exist, but their software imple-
mentation is often not public, or it is a part of a larger software package and is
able to solve only those cases, which are applicable in that particular area [11].
One of the more general ones is the package FISHPACK[12] which solves the
second order finite difference approximation of the Poisson or Helmholtz equa-
tion on rectangular grids. Its origin predates FORTRAN 77 and although it has
been updated in 2004 to version 5.0 to be compatible with Fortran 90 compilers,
the non-existent parallel version, the remaining non-standard features and
missing interfaces to other programming languages make it obsolete.

This paper presents the free software implementation of a fast direct solver
for the Poisson equation in 1, 2 and 3 dimensions with several types of boundary
conditions and with both the pseudo-spectral and the finite difference approx-
imation. The solver is called PoisFFT. Section 2 contains the overview of the
methods used to solve the Poisson equations in PoisFFT. Section 3 briefly in-
troduces the software implementation and its performance is tested in Section
4. In Section 5 we present the application of the Poisson solver to the solution
of the incompressible flow.

2. Solution methods

2.1. Pseudo-spectral method

The first type of approximation PoisFFT solves is the pseudo-spectral method
approximation which is achieved by decomposing the continuous problem us-
ing the Fourier series and solving it in the frequency domain. Consider the 1D
Poisson problem (1) on interval \([0, L]\). With periodic boundary conditions any
sufficiently smooth function \(f\) on this interval can be decomposed as

\[
\hat{f}(x) = \sum_{k=-\infty}^{\infty} \tilde{f}_k e^{2\pi i x/L},
\]

where the complex coefficients are computed as
2.1 Pseudo-spectral method

\[ \hat{f}_k = \frac{1}{L} \int_0^L f(x)e^{-2\pi i k x/L} dx. \]  \hspace{1cm} (3)

After substituting from (2) for \( \varphi \) and \( g \) we get

\[ -\left( \frac{2\pi k}{L} \right)^2 \hat{\varphi}_k = \hat{g}_k, \quad \forall k, \]  \hspace{1cm} (4)

which can be used to compute the solution in the basis of the Fourier modes. The modes \( e^{2\pi i k x/L} \) are eigenvectors of the linear operator \( \frac{\partial^2}{\partial x^2} \) with the eigenvalues \( \lambda_k = -\left( \frac{2\pi k}{L} \right)^2 \).

In the pseudo-spectral method the solution and the source term are evaluated on a grid of points. Consider a uniform grid of \( n + 1 \) points

\[ x_i = i \frac{L}{n}, \quad i = 0 \ldots n. \]  \hspace{1cm} (5)

Due to the periodic boundary conditions we can consider only \( n \) points during the computations

\[ f_n = f(x_n) = f(x_0) = f_0. \]  \hspace{1cm} (6)

The point values \( f_i \) can be transformed using

\[ f_j = \sum_{k=0}^{n-1} \hat{f}_k e^{2\pi i k j/n}, \]  \hspace{1cm} (7)

\[ \hat{f}_k = \frac{1}{n} \sum_{j=0}^{n-1} f_j e^{-2\pi i k j/n}. \]  \hspace{1cm} (8)

The equation 8 is the discrete Fourier transform (DFT) which is used to compute the coefficients of the vector \( f_j \) in the basis of the discrete Fourier modes \( e^{2\pi i k j/n} \). The equation 7 is the inverse discrete Fourier transform (IDFT) and is used to compute the point values \( f_j \).

The pseudo-spectral approximate solution can be computed using the equation (4) for the coefficients of the discrete Fourier modes on the finite grid.

When the boundary conditions are not periodic, different set of basis functions is used. For the Dirichlet boundary conditions

\[ f = 0 \quad \text{on} \quad \partial \Omega \]  \hspace{1cm} (9)

the Fourier series uses only the real sine functions
2.1 Pseudo-spectral method

\[ f(x) = \sum_{k=1}^{\infty} \hat{f}_k \sin \left( \frac{\pi k x}{L} \right), \quad (10) \]

\[ \hat{f}_k = \frac{2}{L} \int_{0}^{L} f(x) \sin \left( \frac{\pi k x}{L} \right) dx, \quad (11) \]

while for the Dirichlet boundary conditions

\[ \frac{\partial f}{\partial x} = 0 \quad \text{on} \partial \Omega \quad (12) \]

the Fourier series uses only the real cosine functions

\[ f(x) = \hat{f}_0 + \sum_{k=1}^{\infty} \hat{f}_k \cos \left( \frac{\pi k x}{L} \right), \quad (13) \]

\[ \hat{f}_k = \frac{2}{L} \int_{0}^{L} f(x) \cos \left( \frac{\pi k x}{L} \right) dx, \quad (14) \]

and the Fourier coefficients \( \hat{f}_k \) are real numbers.

Also, two different kinds of the uniform grid are possible. The first type of the grid is the regular grid, which in the case of the Dirichlet boundary conditions contains only the internal points

\[ x_j = (j + 1) \frac{L}{n+1}, \quad j = 0 \ldots n-1, \quad (15) \]

whereas in the case of the Neumann boundary conditions it also contains the boundary nodes

\[ x_j = j \frac{L}{n-1}, \quad j = 0 \ldots n-1. \quad (16) \]

The other type is the staggered grid

\[ x_j = \left( j + \frac{1}{2} \right) \frac{L}{n}, \quad j = 0 \ldots n-1. \quad (17) \]

In the pseudo-spectral method on a grid different discrete sine transforms (DST) and discrete cosine transforms (DCT) have to be used depending on the grid and the boundary conditions. They are summarized in Table 1.

Finally the eigenvalues are specified in the same notation as the discrete transform in Table 3. The whole algorithm of the Poisson solver can be summarized as
2.2 Finite difference method

The equation (1) can be discretized using the second order central finite differences

$$\frac{\partial \varphi}{\partial x}(x_j) \simeq \frac{\varphi_{j+1} - 2\varphi_j + \varphi_{j-1}}{(\Delta x)^2},$$  \hspace{1cm} (18)$$

where $\Delta x = x_j - x_{j-1}$. This discretization leads to the system of linear algebraic equations

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**Table 1:** Real discrete Fourier transforms

| DST-I         | $\hat{f}_k = 2 \sum_{j=0}^{n-1} f_j \sin (\pi(j + 1)(k + 1)/(n + 1))$ |
|---------------|-------------------------------------------------------------------------|
| DST-II        | $\hat{f}_k = 2 \sum_{j=0}^{n-1} f_j \sin (\pi(j + 1/2)(k + 1)/n)$         |
| DST-III       | $\hat{f}_k = (-1)^k f_{n-1} + 2 \sum_{j=0}^{n-2} f_j \sin (\pi(j + 1)(k + 1/2)/n)$ |
| DCT-I         | $\hat{f}_k = f_0 + (-1)^k f_{n-1} + 2 \sum_{j=1}^{n-1} f_j \cos (\pi j k/(n - 1))$ |
| DCT-II        | $\hat{f}_k = 2 \sum_{j=0}^{n-1} f_j \cos (\pi(j + 1/2)k/n)$               |
| DCT-III       | $\hat{f}_k = f_0 + 2 \sum_{j=1}^{n-1} f_j \cos (\pi j (k + 1/2)/n)$       |

**Table 2:** Discrete Fourier transforms used in the Poisson solver

| boundary conditions | grid     | forward | backward |
|---------------------|----------|---------|----------|
| periodic            | regular  | DFT     | IDFT     |
| Dirichlet           | regular  | DST-I   | $\frac{1}{2n+1}$ DST-I |
| Dirichlet           | staggered| DST-II  | $\frac{1}{2n}$ DST-III |
| Neumann             | regular  | DCT-I   | $\frac{1}{2n}$ DCT-I   |
| Neumann             | staggered| DCT-II  | $\frac{1}{2n}$ DCT-III |

1. Compute the coefficients of the right-hand side $g$ in the basis of eigenvectors of the discrete Laplacian using the forward discrete transforms in Table 2.

2. Compute the solution in this basis by dividing the coefficients by the eigenvalues in Table 3.

3. Transform the solution back to the basis of the grid point values using the backward transforms in Table 2.

The efficiency of this algorithm comes from the possibility of using the Fast Fourier Transform (FFT) to perform the discrete transforms.
Table 3: The eigenvalues for the eigenvectors corresponding to the transforms in Table 2 in the pseudo-spectral approximation

| boundary conditions | grid     | eigenvalues                                      |
|---------------------|----------|-------------------------------------------------|
| periodic            | regular  | \( \lambda_k = - \left( \frac{2\pi k}{L} \right)^2, \quad k < \lfloor n/2 \rfloor - 1 \) \[ \lambda_k = - \left( \frac{2\pi(n-k)}{L} \right)^2, \quad k \geq \lfloor n/2 \rfloor - 1 \] |
| Dirichlet           | regular  | \( \lambda_k = - \left( \frac{\pi(k+1)}{L} \right)^2 \) |
| Dirichlet           | staggered| \( \lambda_k = - \left( \frac{\pi(k+1)}{L} \right)^2 \) |
| Neumann             | regular  | \( \lambda_k = - \left( \frac{\pi k}{L} \right)^2 \) |
| Neumann             | staggered| \( \lambda_k = - \left( \frac{\pi k}{L} \right)^2 \) |

\[
L \varphi = g, \tag{19}
\]

where \( L \) is the matrix resulting from the discretization (18) and from the boundary conditions. As reviewed by Schumann and Sweet [9] the eigenvectors of matrix \( L \) are those used in the discrete transforms in Table 2 with eigenvalues summarized in Table 4.

The algorithm for the solution of the algebraic system (19) is therefore equivalent to the algorithm for the pseudo-spectral approximation in Section 2.1 with a different set of eigenvalues.

2.3. Multiple dimensions

If the boundary conditions on all domain boundaries are equal, the extension of the algorithm to multidimensional problems is straightforward. The multidimensional discrete Fourier transforms are defined as separable products of the one dimensional transforms. For example, for the periodic boundary conditions in 3D the following transform can be used

\[
f_{j_1 j_2 j_3} = \sum_{k_1=0}^{n_1-1} e^{2\pi i k_1 j_1/n_1} \sum_{k_2=0}^{n_2-1} e^{2\pi i k_2 j_2/n_2} \sum_{k_3=0}^{n_3-1} \hat{f}_{k_1 k_2 k_3} e^{2\pi i k_3 j_3/n_3}, \tag{20}
\]

\[
\hat{f}_{k_1 k_2 k_3} = \frac{1}{n_1 n_2 n_3} \sum_{j_1=0}^{n_1-1} e^{-2\pi i k_1 j_1/n_1} \sum_{j_2=0}^{n_2-1} e^{-2\pi i k_2 j_2/n_2} \sum_{j_3=0}^{n_3-1} f_{j_1 j_2 j_3} e^{-2\pi i k_3 j_3/n_3}. \tag{21}
\]

Efficient multidimensional versions of the discrete transforms are commonly included in the FFT libraries. Similar process can be used when the boundary
Table 4: The eigenvalues for the eigenvectors corresponding to the transforms in Table 2 in the second order central finite difference approximation according to Schumann and Sweet [9]

| boundary conditions | grid       | eigenvalues                                      |
|---------------------|------------|--------------------------------------------------|
| periodic            | regular    | \( \lambda_k = - \left( \frac{2 \sin \left( \frac{k \pi}{n} \right)}{\Delta x} \right)^2 \) |
| Dirichlet           | regular    | \( \lambda_k = - \left( \frac{2 \sin \left( \frac{\pi(k+1)}{2(n+1)} \right)}{\Delta x} \right)^2 \) |
| Dirichlet           | staggered  | \( \lambda_k = - \left( \frac{2 \sin \left( \frac{\pi (k+1)}{2n} \right)}{\Delta x} \right)^2 \) |
| Neumann             | regular    | \( \lambda_k = - \left( \frac{2 \sin \left( \frac{\pi k}{2(n-1)} \right)}{\Delta x} \right)^2 \) |
| Neumann             | staggered  | \( \lambda_k = - \left( \frac{2 \sin \left( \frac{\pi k}{2n} \right)}{\Delta x} \right)^2 \) |

conditions differ, as shown for the combination of the periodic and the staggered Neumann boundary conditions by Wilhelmson and Ericksen [6]. It is then necessary to use a sequence of transforms of smaller dimension.

The eigenvalues of the discrete 3D Laplace operator associated with the Fourier mode \( \hat{f}_{k_1, k_2, k_3} \) are computed from the one dimensional eigenvalues as

\[
\lambda_{k_1, k_2, k_3} = \lambda_{k_1} + \lambda_{k_2} + \lambda_{k_3}.
\] (22)

3. Software implementation

The fast Poisson solver PoisFFT is a library written in Fortran 2003 with bindings to C, C++ and Python. It uses the FFTW3[13] library for the discrete Fourier transforms and the PFFT[14] library for the MPI parallelization of FFTW3 transforms. It is distributed as a free software with the GNU GPLv3 license, which also covers FFTW3 and PFFT. The solver objects in PoisFFT are available in Fortran as separate derived types in the IEEE single of and double precision and as a class template in C++.

The library is parallelized using OpenMP for shared memory computers and using MPI for distributed memory computers (e.g., clusters). Combination of OpenMP and MPI at the same time is not implemented. It can also employ the internal FFTW parallelization using POSIX threads. The MPI version of the library uses the PFFT library to partition the 3D grid using a 2D decomposition along the last two dimensions in Fortran (along the first two dimensions in C) as shown in Fig. 1.

PoisFFT can solve the Poisson equation in 1, 2 and 3 dimensions with any of the boundary conditions presented in Section 2 provided all domain boundaries use the same boundary condition. Because of practical applications in
geophysical fluid dynamics, particularly in the computational fluid dynamics model CLMM (Section 5); the combination of the periodic boundary condition in the horizontal directions and the staggered Neumann boundary condition in the vertical is also implemented. In this case the parallel real 1D transform is not available in FFTW3 or PFFT and we parallelized this step using a global array transpose via the subroutine \texttt{MPI\_Alltoallv()} and local array transposes.

4. Performance evaluation

Due to the differences in the discrete Fourier transforms for different boundary conditions, the wall-clock times and the CPU times necessary for the solution of the Poisson equation depend on the boundary conditions. We chose the 3D solvers with the periodic boundary conditions and the Neumann boundary conditions on the staggered grid to test the solver with the 3D complex transform and with the 3D real transform.

All tests were performed at the cluster \texttt{zapat.cerit-sc.cz} at the Czech supercomputing center Cerit-SC. The computational nodes contained 2 sockets with 8-core Intel E5-2670 2.6GHz processors and 128 GB RAM and were connected using an InfiniBand network. PoisFFT was compiled with the Intel Fortran compiler 14.1 and linked with OpenMPI 1.8.

The first test examined the strong scaling on a fixed domain with 512 points in every dimension. The same problem was solved with an increasing number of CPU cores. From the measured times in Fig. 2 it is clear that the OpenMP version, which directly calls FFTW, is considerably faster than the MPI version, which calls the PFFT wrapper over FFTW and which has to perform significant amount of message passing between processes. However, OpenMP is limited to single node on the cluster used for the computations. One can also notice a decrease of efficiency when going from 16 to 32 cores. One node has 16 cores and the expensive network memory transfers slow the computation when more nodes are needed.

For the weak scaling test we used a domain discretization in which the number of points increased with the number of CPU cores. There were 256 points...
in each dimension per core. The complete problem size was therefore proportional to the number of cores. The results of the time measurements are in Fig. 3. They are consistent with the scaling $O(N \ln(N))$ which holds for the FFT transforms[13].

5. Application of PoisFFT to simulation of incompressible flow

5.1. Model CLMM

Originally, PoisFFT was developed to support the atmospheric computational fluid dynamics code CLMM (Charles University Large-Eddy Microscale Model)[15]. This model simulates atmospheric flows using the incompressible Navier-Stokes equations with an eddy viscosity subgrid model.

The incompressible Navier-Stokes equations are
where $u$ is the velocity vector, $p$ is the pressure and $\nu_{sgs}$ is the eddy viscosity modeled according to Nicoud et al. [16]. The equations (23–24) do not contain an evolution equation for pressure. The model CLMM uses the projection method[1] and the 3 stage Runge-Kutta method[17]

\[
\frac{\partial u}{\partial t} + \nabla \cdot (uu) = -\nabla p + \nu_{sgs} \nabla^2 u,
\]

(23)

\[
\nabla \cdot u = 0,
\]

(24)

\[
\begin{align*}
\mathbf{u}^{(1)} &= \mathbf{u}^{n}, \\
p^{(1)} &= p^{n-1/2}, \\
\frac{\mathbf{u}^{*} - \mathbf{u}^{(k)}}{\Delta t} &= -\alpha_k \nabla p^{(k)} + \gamma_k \left( -\nabla \cdot (\mathbf{u}^{(k)} \mathbf{u}^{(k)}) + \nu \nabla^2 \mathbf{u}^{(k)} \right) + \\
&+ \zeta_k \left( -\nabla \cdot (\mathbf{u}^{(k-1)} \mathbf{u}^{(k-1)}) + \nu \nabla^2 \mathbf{u}^{(k-1)} \right) \\
\nabla^2 \phi &= \frac{\nabla \mathbf{u}^{*}}{\alpha_k \Delta t}, \\
\frac{\mathbf{u}^{(k+1)} - \mathbf{u}^{*}}{\alpha_k \Delta t} &= -\nabla \phi, \\
p^{(k+1)} &= p^{(k)} + \phi, \\
&\text{for } k = 1..3, \text{ and} \\
\mathbf{u}^{n+1} &= \mathbf{u}^{(4)}, p^{n+1/2} = p^{(4)},
\end{align*}
\]

(25–30)

with the set of coefficients

\[
\begin{align*}
\alpha_1 &= \frac{8}{15}, \quad \alpha_2 = \frac{2}{15}, \quad \alpha_3 = \frac{1}{3}, \\
\gamma_1 &= \frac{8}{15}, \quad \gamma_2 = \frac{5}{12}, \quad \gamma_3 = \frac{3}{4}, \\
\zeta_1 &= 0, \quad \zeta_2 = -\frac{17}{60}, \quad \zeta_3 = -\frac{5}{12}.
\end{align*}
\]

(31)

The spatial derivatives in equations (25–30) are discretized using the second order central finite differences on a staggered grid[18] with the exception of the advective terms $-\nabla \cdot (uu)$ for which fourth order central differences are used.

In every Runge-Kutta stage first a predictor velocity field $\mathbf{u}^{*}$ is computed and afterward it is corrected to be divergence free. The discrete Poisson problem (27) must be solved in the corrector step, with the staggered Neumann boundary conditions on all outside boundaries except the boundaries where the periodic boundary condition for the velocity are imposed and where the periodic condition applies to the discrete Poisson equation as well.

It is possible to use this model on the uniform grid to simulate complex geometries thanks to the immersed boundary method (IBM)[19], which introduces
5.2 Performance test

To evaluate the effect of CLMM we chose the test case defined by the COST Action ES1006 “Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments” with a virtual city called Michelstadt which serves for validation of models for flow and dispersion in urban environments[21]. The description of the geometry and the flow validation data are available at the CEDVAL-LES website\(^1\). In this paper only the velocity field is simulated for a direct comparison of the relative performance of the Poisson solver PoisFFT and other parts of the model.

The computational domain of the Michelstadt city had dimensions 1326 m \(\times\) 836 m \(\times\) 399 m and was discretized using a constant resolution of 3m in all directions leading to the total number of 16.3 million cells. The performance was measured for the first 100 time-steps for different parallel setups – OpenMP and MPI – with different numbers of CPU cores. The fastest configuration was used to compute the flow for 10000 s of the real scale time and the average flow and turbulence was compared to the experimental values. The performance was tested on the cluster \texttt{luna.fzu.cz} in the Czech national grid MetaCentrum. The computational nodes have 2 sockets with the 8-core Intel Xeon E5-2650 2.6 Ghz CPU, 96 GB of RAM and are connected using an InfiniBand network.

The scaling of the wall-clock time for the solution of first 100 time-steps is in Fig. 4. Although the MPI version of PoisFFT is slower than the OpenMP version for the same number of CPU cores, the whole model CLMM is as fast with MPI as with OpenMP on the used nodes up to 8 threads. The OpenMP version with 16 threads is slower than the MPI version with 16 processes. CLMM in its finite difference parts to benefit from the improved data locality in the

\(^1\)\url{http://www.mi.uni-hamburg.de/CEDVAL-LES-V.6332.0.html}, accessed on September 28th, 2014.
distributed MPI version. The relative contribution of PoisFFT to the total CLMM solution time is between 22% – 36% when using MPI. When using OpenMP the PoisFFT portion starts at 20% for one and two threads and decreases for higher numbers of threads as the parallel efficiency of CLMM in OpenMP decreases. From these ratios it is clear that the efficient Poisson solver is a necessity for an efficient computation and that PoisFFT scales well enough so that it doesn’t become a bottleneck at the moderate numbers of cores used for the test.

The correctness of the computation was evaluated by comparison of the time-averaged simulated wind field with the measurements. Fig. 5 shows the comparison of the values of the velocity components in the reference points of CEDVAL-LES. An illustration of the simulated wind field at height 7.5 m above the ground is in Fig. 6.

6. Conclusions

The fast Poisson solver PoisFFT is be able to compute a discrete approximate solution to the Poisson equation in the pseudo-spectral or second order finite difference approximation. It is parallel using OpenMP and MPI and the parallel scaling was demonstrated to be usable for moderate numbers of CPU cores. The scaling for the number of cores in the order of thousands remain untested due to the lack of suitable hardware. The experiments of Pippig [14] with the underlying PFFT library suggest that the the solver could scale even for large numbers of cores.

It was demonstrated that PoisFFT can be employed for the solution of the discrete Poisson equation in the projection step in an incompressible flow solver. It does not become a bottleneck at 128 cores and it is expected to scale well even further.

The library can be used from Fortran, C and C++. Interfaces to other computer languages (e.g., Python) are planned.
Figure 6: The Michelstadt geometry with the instantaneous field of the wind velocity magnitude at height 7.5 m above ground. The blue, green and red buildings are 15, 18 and 24 m high, respectively.

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