

Welcome

Dear participants,

welcome to the Fourth deal.II Users' and Developers' Workshop at Texas A&M University. After the great success of the previous deal.II workshops in Heidelberg in 2010 and 2012, we decided to organize a new iteration of it. The aim of this workshop is to bring together experts, researchers, and students using deal.II.

This workshop is a platform for making contact and exchanging ideas in the field of scientific computing with the software library deal.II. The library has evolved a lot over the last few years and this meeting gives the opportunity to sustain this development. You can learn about new features of the library, you can present your own progress with the help of deal.II, and, finally, you can discuss topics about the new development of deal.II itself.

We will not only have presentations, but we have time slots for discussions and *code jams* (see page 17). This mixture has been very successful in the past years and we hope that you are as excited to contribute as we are.

Apart from the scientific program, we will have a conference dinner on Tuesday evening at 6 pm at the restaurant La Bodega in College Station, TX.

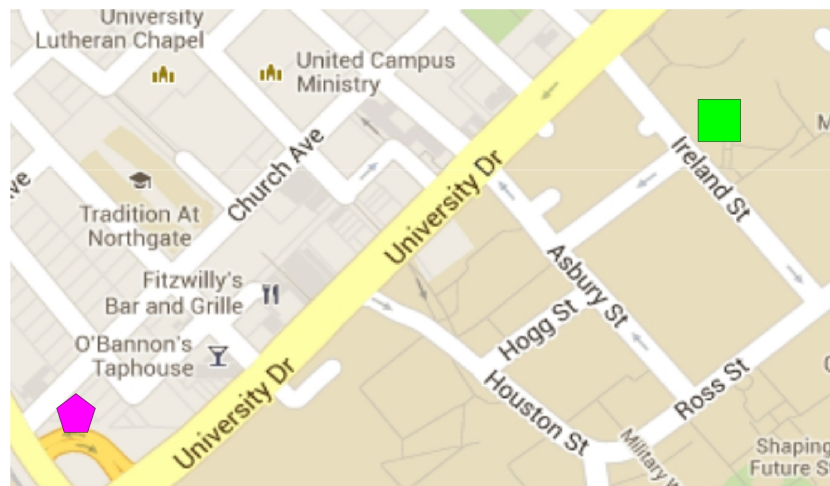
We wish everybody fruitful discussions and an enjoyable workshop!

The organizers:

Markus, Timo, Matthias, and Wolfgang



- Super 8 Hotel
- Blocker Building
- ◆ La Bodega



(source: maps.google.com)

Time table

| | Monday | Tuesday |
|----------|------------------------------------|---------------------------------|
| 09:00 am | 09:00 am Registration | 09:00 am Timo Heister (9) |
| | 09:15 am Opening Remarks | |
| | 09:30 am Wolfgang Bangerth (1) | 09:30 am Bruno Turcksin (10) |
| 10:00 am | 10:00 am Martin Kronbichler (2) | 10:00 am Coffee break |
| | 10:30 am Coffee break | 10:30 am Daniel Arndt (11) |
| 11:00 am | 11:00 am Sarah Stamps (3) | 11:00 am Marek Čapek (12) |
| | 11:30 am Seshu Tirupathi (4) | 11:30 am Sanghyun Lee (13) |
| 12:00 pm | 12:00 pm Chih-Che Chueh (5) | 12:00 pm Lunch break |
| | 12:30 pm Lunch break | |
| 01:00 pm | | 01:30 pm Daniel Brauss (14) |
| 02:00 pm | 02:00 pm Jörg Frohne (6) | 02:00 pm Marc Secanell (15) |
| | 02:30 pm Bärbel Janssen (7) | 02:30 pm Matthias Maier (16) |
| 03:00 pm | 03:00 pm Yan Yan (8) | 03:00 pm Coffee break |
| | 03:30 pm Coffee break | |
| 04:00 pm | 04:00 pm Discussion | 03:45 pm Luca Heltai (17) |
| | | 04:15 pm Jason Sheldon (18) |
| 05:00 pm | | 04:45 pm Thomas Wick (19) |

| Wednesday | Thursday |
|---------------------------------|--------------------------|
| 09:00 am Guido Kanschat (20) | 09:00 am Code jam |
| 09:30 am Matthias Maier (21) | |
| 10:00 am Coffee break | 10:15 am Coffee break |
| 10:30 am Code Jam | 10:45 am Code jam |
| 12:15 pm Lunch break | 12:15 pm Lunch break |
| 02:00 pm Closing Remarks | 02:00 pm Code jam |
| 02:15 pm Discussion | |
| 03:15 pm Coffee break | |
| 03:45 pm Code Jam | |

Abstracts

The talks are listed in session order and the numbers correspond to the numbers in the schedule.

1. Past and Future of deal.II

Wolfgang Bangerth (*Texas A&M University*)

Over the past 15 years, the deal.II project has morphed from an in-house code to an open source software with contributors from around the world. I will briefly review where we are coming from, describe where we are, and what I see as the challenges we will need to address in the future. I will also briefly hit upon a few of the topics that will be the subject of later talks throughout the workshop.

2. Efficient Matrix-Free Methods in deal.II

Martin Kronbichler (*Technische Universität München*)

I present the matrix-free capabilities recently added to deal.II by Katharina Kormann and me, including tutorial programs step-37 and step-48. The framework allows for very fast operations, typically between ten and hundred times faster than standard deal.II assembly routines. For quadratic elements and higher, matrix-free matrix-vector products are also considerably faster than sparse matrix-vector products. This advantage is because of less memory transfer at low order and also less operations at high order. Even more, I expect this advantage to become more pronounced on future computer architectures.

The matrix-free implementation uses parallelism on three levels: MPI parallelism with the `parallel::distributed::Vector` class, thread parallelism with advanced task scheduling, and vectorization. The high performance gain compared to usual assembly is due to four specific design choices: vectorization is realized by working on several cells at a time (using an array-of-struct-of-arrays data layout); the loop over cells is represented by a task dependency graph that avoids writing to the same vector entries by several threads; vector indices and constraints are transformed to process-local index space for direct array access; compile-time information of the element kernel in terms of the element degree. The matrix-free design currently re-implements several things already present in deal.II in a more efficient but less general way. As it would be desirable to connect this more closely to other parts of the library, I will discuss possible ways for doing so.

3. Kinematic and Dynamics of the East African Rift: System-Wide Results and Research Outlook for Rift-Scale Processes

Sarah Stamps (*Massachusetts Institute of Technology (MIT)*)

The Nubian and Somalian plates actively diverge along the East African Rift System (EARS), which straddles >1000 km high plateaus. The competing role of horizontal mantle tractions and gravitational potential energy gradients in driving this system is a long-standing debate. At the system-wide scale we model lithospheric dynamics and test the role of mantle shear with two independent finite element techniques. By comparing calculated velocities with well-constrained GPS velocities along the EARS and on the Somalian plate we find gravitational potential energy gradients dominate the force-balance driving Nubia-Somalia divergence. At the scale of individual rift-segments weakening mechanisms, such as magmatism, lithospheric removal, and the reactivation of pre-existing structures, are necessary to overcome the strength of the lithosphere and initiate rapture. These processes, and perhaps others, may induce deformation that is inconsistent with traditional models of rift-perpendicular opening of continental rifts. A developing GPS velocity field in East Africa measures rift-parallel motions along 3 rift-segments, albeit with large uncertainties. In this work we will (1) re-measure geodetic benchmarks in East Africa where rift-parallel deformation is detected, (2) develop kinematic models for each rift-segment, and (3) test multiple rift-parallel deformation hypotheses with numerical models utilizing deal.II.

4. Numerical Study of Melt Migration in an Upwelling Heterogeneous Mantle

Seshu Tirupathi (*Brown University*)

Generation and segregation of magma in the Earth and planetary interior has been a subject of intensive studies in the Earth Science community. In particular, Orthopyroxene-free dunite channels have been frequently observed in mantle sections of ophiolites. One of the proposed theories to explain this phenomenon is the dissolution of pyroxene when olivine-normative basalts percolate through a partially molten mantle. In this presentation, I'll talk about developing an efficient and accurate numerical model using Discontinuous Galerkin methods that can be used to study the interaction between the melt and solid mantle during melt migration.

5. Integrated Numerical Methods for Transient Two-Phase Flow with Capillary and Gravity Effects in Porous Media

Chih-Che Chueh (*Queen's University*)

The simulation of multiphase flow in porous media is a ubiquitous problem in a wide variety of fields, such as fuel cell modeling, oil reservoir simulation, magma dynamics, or tumor modeling. However, it is computationally expensive. This presentation presents an interconnected set of algorithms which we show can accelerate computations by more than two orders of magnitude compared to traditional techniques, yet retains the high accuracy necessary for practical applications. Specifically, we base our approach on a new adaptive operator splitting technique driven by an a posteriori criterion to separate the flow from the transport equations; adaptive meshing to reduce the size of the discretized problem; efficient block preconditioned solver techniques for fast solution of the discrete equations; and a recently developed artificial diffusion strategy to stabilize the numerical solution of the transport equation. Recently, the work has been extended to perform 3D simulations including a massive implementation parallelization and enhanced physical modelling, such as capillary diffusion and gravity, that enhance the applicability of the method to a broader range of multi-phase transport problems of practical interest.

6. Efficient Large-Scale Parallel Solution of Thermomechanical Contact Problems

Jörg Frohne (*Technische Universität Dortmund*)

Our talk will treat two topics which will be joined in a model with the aim to simulate a deep hole drilling process. First we introduce a thermomechanical problem which describes elasto-plastic deformations with hardening coupled with a heat equation. After a brief introduction of the model and the variational equations we propose an integrated set of computational methods based on the finite element method for the large-scale parallel solution. Some results for three dimensional examples will demonstrate the efficiency of this approach. To discretize our problem we use piecewise linear or quadratic ansatz functions on a h-adaptive refined mesh. In the second part we present an intuitive way to handle mesh separation e.g. caused by the cutting edge of the drill using a Discontinuous Galerkin (DG) method and reasonable physical criteria for the separation along an edge of an element. To enforce continuity between the DG elements as well as the Dirichlet boundary conditions we apply a Nitsche method. Of course this approach leads to a bigger amount of unknowns compared to a continuous approach but which can be reduced by using the DG elements only in a specific area around the separation zone. Since we treat the contact conditions with a primal dual active set method we have to think about if it is admissible to use DG elements along the contact boundary without losing the biorthogonality property. Finally we present some first results and an outlook.

This is joint work with Heribert Blum, Andreas Rademacher, and Korosh Taebi from Technische Universität Dortmund.

7. The hp -Adaptive Galerkin Time Stepping Method for Nonlinear Differential Equations with Finite Time Blow-Up

Bärbel Janssen (*KTH Royal Institute of Technology*)

Originally the problem of interest would be

$$u_t = \Delta\phi(u) + Q(u), \quad t > 0, x \in \Omega$$

with boundary and initial conditions. This could be a model for heat outflow from the domain Ω , in which diffusion and combustion processes take place. The magnitude of heat loss depends on the intensity of combustion inside Ω . We are interested in dealing with the blow-up in finite time. So we restrict the problem to

$$u_t = Q(u), \quad u(0) = u_0.$$

In this talk we will present hp -adaptive Galerkin methods in time to resolve the blow-up. Existence of solutions are shown by fixed point arguments and reconstruction techniques. To resolve the blow-up well, we use adaptivity and local mesh refinement based on DWR techniques. Using Sobolev embeddings we are able to decide whether to refine in h or p .

8. Optimal Control of Conjugate Heat Transfer Problems

Yan Yan (*Columbia University*)

This work outlines the first step towards the development of practical optimal control algorithms for the conjugate heat transfer (CHT) process. Conjugate heat transfer represents the physical process, in which the fluid is the carrier of thermal energy, convectively transporting heat from the conjugate heating device. Conjugate heat transfer problems have many important industrial applications, such as the heat exchange process in power plants and the cooling process in electronic packaging industry, and they have been hot research topics in thermal science for many years. The optimal control of CHT processes has been quite computationally challenging. First, the CHT process is a multiphysics system and highly nonlinear, this makes the optimization problem on top nonconvex and nonlinear. Second, once discretized, the governing equations of the CHT process can easily scale up to millions of degrees of freedom (DOF). This renders the control problem very large scale. Third, like many other PDE constrained optimization problems, the separation between the state and the control (or design) variables has demanded careful consideration for calculating the gradient of the objective function. All these three aspects have made the general-purpose optimization software not suitable. In this presentation, we show some recent results and demonstrate the feasibility and effectiveness of our numerical schemes via recovering the boundary control profile of Poiseuille flow.

9. Parallel Linear Algebra in deal.II

Timo Heister (*Clemson University*)

I will give an introduction into parallel computations using deal.II and how to use Trilinos or PETSc for the linear algebra. Recent changes allow writing programs that work with either by changing only a single line of code.

10. Large Parallel Computation

Bruno Turcksin (*Texas A&M University*)

Up to version 7.3 of deal.II, the degrees of freedom (which are uniquely defined) were stored using unsigned int datatype. This limited the number of degrees of freedom to four billion. When deal.II was used in conjunction with PETSc or Trilinos, this number was divided by two (PETSc and Trilinos use integer indices). To increase the number of unknowns that can be solved using deal.II, the degrees of freedom are now stored using long long int (64 bit indices) and the new 64 bit capabilities of Epetra (Trilinos) are employed. The new version of deal.II is completely compatible with the previous version and can be compiled to use 32 or 64 bit indices indifferently.

11. $\mathcal{Q}_k + \mathcal{Q}_0$ -Elements in Incompressible Flows

Daniel Arndt (*Universität Göttingen*)

It is well-known that in finite element discretizations of incompressible flow problems the numerical solution is in general not pointwise solenoidal, unless the divergence of the velocity ansatz space is contained in the pressure ansatz space. Although many models are based on the conservation of mass, in discretizations often finite elements are used that are not divergence free.

In this talk, we consider the augmented Taylor-Hood pair $\mathcal{Q}_k/(\mathcal{Q}_{k-1} + \mathcal{Q}_0)$ that improves conservation of mass. We examine the inf-sup stability of this discretization for quadrilateral and hexahedral meshes. After presenting convergence results for the Stokes problem, we discuss some details on the implementation of these elements in deal.II and on the numerical costs for the additional discontinuous degree of freedom. Finally, a turbulent channel flow is considered as a test case for the Navier-Stokes equations and we examine how the improved mass conservation influences the quality of the numerical solution.

12. Blood Flow Modeling

Marek Čapek (*Univerzita Karlova v Praze*)

We model blood as a polymer-like liquid. We follow the developments of microstructure-based modelling of blood of Owens and coworkers. Shear-thinning property of blood is caused by the creation of column-like structures at low shear-rate. These structures, rouleaux, are in the model represented as dumbbells with different lengths corresponding to different number of red blood cells in rouleaux.

The resulting set of governing equations contains equations for elastic part of stress tensor, which are similar in form to maxwell/oldroyd like fluid. The system contains also an equation for time development of rouleaux size.

We try to implement different strategies for coping with the resulting discrete system of equations. We want to write scalable parallel code, as computations of the model in nontrivial geometries are very demanding on computational time. This parallelization relies on MPI/Petsc features of deal.ii library.

13. Numerical Simulations of the Kaye Effect

Sanghyun Lee (*Texas A&M University*)

The fascinating phenomenon of a leaping shampoo stream, Kaye effect, is a property of non-Newtonian fluid which was first described by Alan Kaye in 1963. It manifest itself, when a thin stream of non-Newtonian fluid is poured into a dish of the fluid. As pouring proceeds, a small stream of liquid occasionally leaps upward from the heap. Since there is no mathematical model or numerical simulation studied before, as a first approach, we have studied a mathematical model and algorithm to find the range of parameters to observe the Kaye effects. In this context we propose a modified projection method for Navier-Stokes equation with open boundary, level set method for free boundary and adaptivity.

Also, in earlier studies it has been debated whether non-Newtonian effects are the underlying cause of this phenomenon, making the jet glide on top of a shear-thinning liquid layer, or whether an entrained air layer is responsible. Here in we show that the jet slides on a lubricating air layer with numerical simulation which is the identical result that we observe from physical experiments.

This is joint work with A. Bonito and J.L. Guermond.

14. Implementation of a Parallel Iterative Solution Method for a Set of MHD Equations

Daniel Brauss (*Auburn University*)

The magnetohydrodynamic equations (MHD equations) have been used to model a wide range of applications in engineering and physics, such as, thermonuclear fusion, liquid metal cooling of nuclear reactors, sea-water propulsion devices, and solidification processes used in the metal and silicon wafer industry. A novel form of the MHD equations has been studied here at Auburn University (existence and uniqueness of solution of these equations have been shown). This study is being continued and current efforts include the implementation of an efficient parallel finite element method to approximate the solution to these equations.

Sufficiently accurate numerical approximations of the solution require solving a system of equations having millions of unknowns. To obtain an approximate solution with a reasonable convergence tolerance we use deal.ii with parallel processing and an iterative solution strategy. In this talk, we summarize the existence and uniqueness results, we review the iterative solution method for the MHD equations, and we discuss the parallel implementation of the method.

15. OpenFCST: Fuel Cell Simulation Toolbox

Marc Secanell (*University of Alberta*)

The Fuel Cell Simulation Toolbox (FCST) is an open-source mathematical modelling package for polymer electrolyte fuel cells. FCST builds on top of the open-source finite element libraries deal.II. It therefore uses many of its classes for discretization and solution of the fuel cell governing equations. FCST has been developed as a modular toolbox from which you can develop your own applications. It contains a build-in fuel cell mesh generator. It can also import quadrilateral meshes generated with the open-source pre-processor Salome. For analysis, it contains a database of equations describing the physical phenomena in fuel cells, a database of fuel cell layer and material properties, and a database with electrochemical reaction kinetic models. The physics and material database in FCST allow you to setup the governing equations for the most important physical processes that take place in a fuel cell. FCST already implements the weak form for many governing equations that are finally solved using the finite element open-source libraries deal.II. In order to analyze your results, FCST output results to .vtk files that can easily be read with the open-source post-processor Paraview. FCST is also integrated with the design and optimization package Dakota. Therefore, it can be used for design and optimization as well as parameter estimation.

In this presentation, an introduction to the FCST software will be given. The presentation will include a description of the software layout including a description of the different databases within the software and how they are integrated to develop different application. Several applications will then be discussed including the development of finite-element solvers for: a) a non-isothermal, multi- component fuel cell membrane electrode assembly model, b) a porous Navier-Stokes model for fuel cell channels and porous media; and, c) a multi-component gas transport model.

Note: FCST will be available from September 1st 2013 at <http://www.openfcst.org> and it is distributed under the MIT License.

This is joint work with A. Putz from Automotive Fuel Cell Cooperation Corp. and V. Zingan, M. Bhaiya, and P. Wardlaw from University of Alberta.

16. A Posteriori Error Estimation for a Heterogeneous Multiscale Finite Element Method

Matthias Maier (*Universität Heidelberg*)

A big class of modelling problems in physics and engineering is of multiscale character, meaning, that relevant physical processes act on highly different length scales. Due to the huge computational costs that are typically connected with multiscale problems, multiscale schemes were developed to avoid the problem to resolve such problems in full.

Typically, an effective model is solved on a coarse scale and effective parameters are determined with the help of localized sampling problems on a fine scale. However, this introduces significant complexity with respect to sources of error—discretization errors on coarse and fine scale as well as a modelling error for the effective model.

This talk will present a Heterogeneous Multiscale Finite Element scheme for elliptic advection-diffusion problems together with an adaptive framework based on a posteriori error estimation with the help of the Dual Weighted Residual method.

An error splitting will allow for a quantitative error assessment of the different sources of error. Furthermore, a model adaptive approach based on the a posteriori error estimation will be presented.

17. Combining BEM, ALE, DAE, FEM and SUPG in deal.II: Steady and Nonlinear Wave-Ship Interactions

Luca Heltai (*SISSA*)

We present a numerical discretization of the equations of inviscid potential flow for the simulation of three-dimensional, unsteady, and nonlinear water waves generated by a ship hull advancing in water.

The equations of motion are written in a semi-Lagrangian framework, and the resulting integro-differential equations are discretized in space via an adaptive isoparametric collocation boundary element method, and in time via implicit backward differentiation formulas (BDF) with adaptive step size and variable order.

When the velocity of the advancing ship hull is non-negligible, the semi-Lagrangian formulation (also known as Arbitrary Lagrangian Eulerian formulation or ALE) of the free-surface equations contains dominant transport terms which are stabilized with a streamwise upwind Petrov-Galerkin (SUPG) method.

The SUPG stabilization allows automatic and robust adaptation of the spatial discretization with unstructured quadrilateral grids. Some results are presented where we compare our numerical model with experimental available experimental results on benchmark hulls advancing in calm water with fixed sink and trim.

18. A Fair Comparison Technique for Fluid-Structure Interaction Coupling Problems

Jason Sheldon (*Pennsylvania State University*)

The multi-physics simulation of coupled fluid-structure interaction problems, with disjoint fluid and solid domains, requires one to choose a method for enforcing the fluid-structure coupling at the interface between solid and fluid. Currently, there does not exist a satisfactory coupling comparison strategy that allows for conclusions to be drawn with respect to the comparison of computational cost and solution accuracy. Using the deal.ii finite element library, we develop a single numerical framework where all aspects of the FSI computation can be held constant, save for the method in which the coupled nature of the fluid-structure equations is enforced. This enables a fair comparison between coupling methods.

We have chosen the two-dimensional benchmark test problem of Turek and Hron to examine the relative accuracy of the coupling methods studied. Standard material models and numerical discretization techniques are employed in this work, as the focus is not on specific numerical schemes, but rather on creating an environment where coupling strategies can be compared in a fair and quantitative manner.

19. Numerical Simulations of Pressurized and Propagating Fractures using a Phase-Field Approach

Thomas Wick (*University of Texas at Austin*)

In this talk, we present modeling, discretization and simulations of pressurized and propagating cracks in a poro-elastic medium. The method of choice is a novel phase-field model developed by Mikelic/Wheeler/Wick in 2013.

The results are validated by spatial mesh convergence studies, comparison to Sneddon's analytical solutions for two- and three dimensional configurations using a constant pressure, and finally, propagating cracks in both dimensions by increasing the pressure.

The simulations show very promising findings for future directions. In particular, the code is validated with benchmarks from which we infer that modeling and implementation are correct.

20. deal.II and Hybrid Programming

Guido Kanschat (*Universität Heidelberg*)

Modern high performance architectures are characterized through a hierarchy of parallel computing units, from multicore processors, which share memory in a single physical computing node equipped with GPU boards to clusters of thousands of such nodes and heterogeneous networks. The challenge originating from these hardware structures for developers of a general purpose finite element library like deal.II consists in the fact that the gap between achieved and peak performance widens more and more if software structures do not take these into account. Therefore, a balance has to be found between wide applicability of the library and sufficient hardware adaptation. Accordingly, certain structures and algorithms we have grown fond of will have to be replaced by more efficient or robust ones. We discuss the high performance computing support existing in the deal.II library, its limits, and future developments to overcome current deficiencies.

21. A C Make Build System for deal.II

Matthias Maier (*Universität Heidelberg*)

CMake is a popular (especially in scientific computing) cross-platform, open-source build system. It provides native support for all major platforms—Unix/Linux, Windows/Cygwin and Mac OS X—, as well as many IDEs—Eclipse, KDevelop, Code-Blocks, XCode, MSVC. With version 8.0 deal.II will switch its build system from autoconf with custom makefiles completely to CMake.

The first part of this talk is devoted to a short overview of the principal design decisions for the new build system and how deal.II is configured and build with it. Furthermore, fundamental concepts and terminology with respect to CMake will be explained.

In the second part some examples of CMake scripts for user projects will be presented. The examples will range from small one file deal.II projects (such as the example steps) to bigger projects with additional external and internal libraries.

Conference Dinner

The conference dinner will take place at

La Bodega
102 Church Ave College Station, TX.

The dinner starts at 6:00 pm with an informal get together at the restaurant and will then transform into the actual dinner later on.

Organization of the *Code Jam*

Besides the traditional talk sessions from Monday until Wednesday, there will be some code jam sessions on Wednesday and Thursday. The idea of this code jam is pretty simple: We offer a room with internet connection and you do the rest!

We would like to give you the opportunity to collaborate, write code together, sketch out new ideas, ask questions, discuss, present your ideas, look over the shoulders on how others work, or just chat with like-minded others.

Everyone is welcome to join us!

List of Participants

| | |
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| Arndt, Daniel | p. 9 |
| | Universität Göttingen Göttingen, Germany |
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| Brauss, Daniel | p. 11 |
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