Erasmus MC
University Medical Center Rotterdam

HOGESCHOOL ROTTERDAM

Porting Erasmus Computing Grid, (Condor enabled) applications for EDGeS

Erasmus Medical Centre

Hogeschool Rotterdam - CMI

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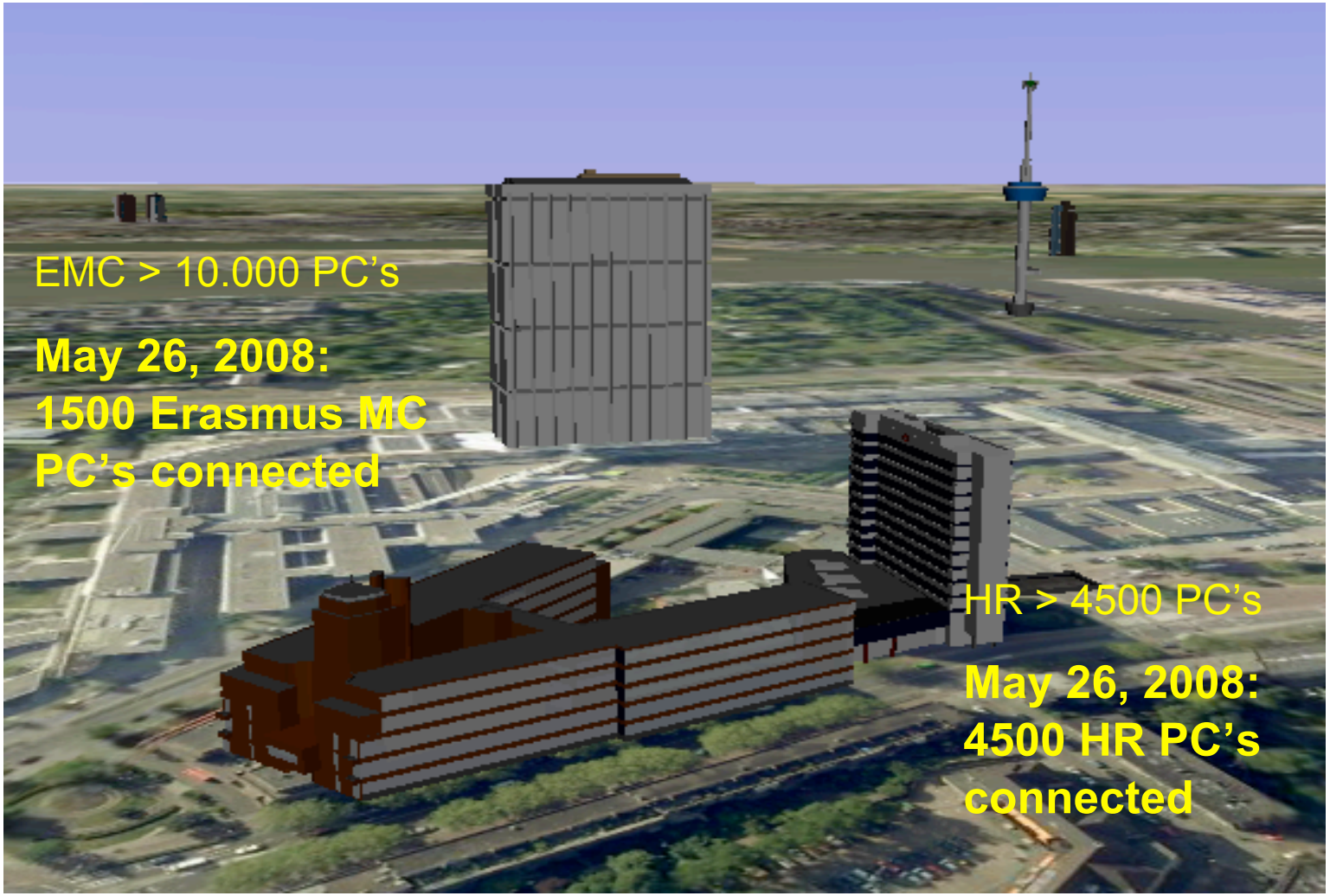
Erasmus Computing Grid



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Objectives
Erasmus Computing Grid

- Using rest and over capacity for socially relevant scientific research.

Teaching:

- Training technicians: building, management and usage of GRID infrastructures.
- Opportunity for GRID related internships.
- Students will be able to use a realistic GRID infrastructure
- Multidisciplinairy GRID related projects.

Mission:

- To make GRIDs well know to as the technology to make better use of computer resources.
- To be an example for other institutions to donate there unused resources for the benefit of science

EDGeS Applications

Genetics/cell biology:

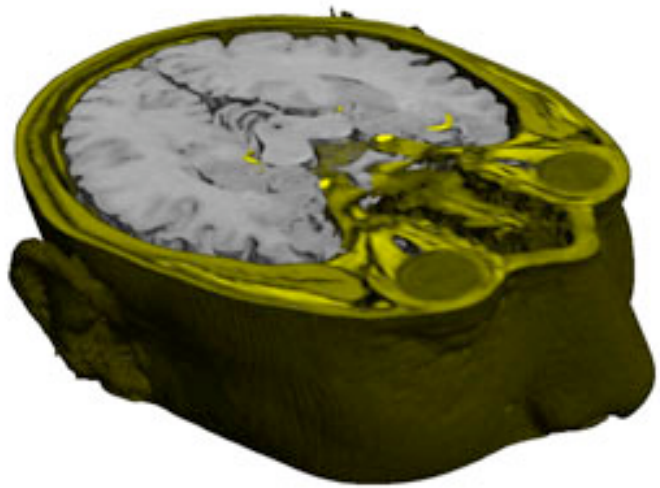
- High-Throughput Sequencing: pipeline analyses
- Sequence comparison
- Simulations of large macromolecular polymer structures

Brain research:

- MRI scan anlyses

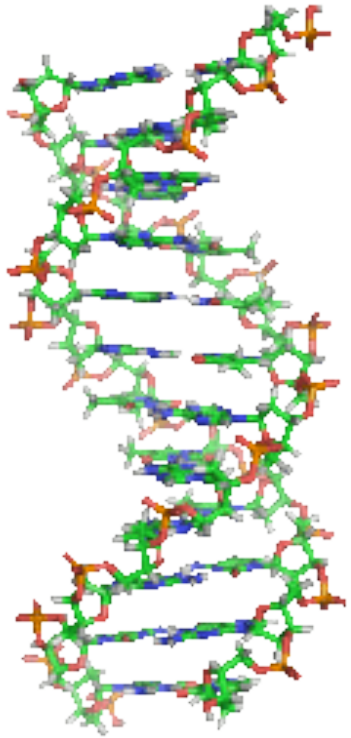
MRI-Morph

MRI-Morph: To understand the differences in brains the Rotterdam Study comprised of ~15,000 participants is taking every second year 3D-MRI scans from these participants. These are analysed and compared by MRI-Morph. From the results correlations are made to other information provided by the Rotterdam Study. The impact of this analysis is of major importance for basic research to understand brain function in general and beyond in diagnostic and treatment in relation to disease. Since the Rotterdam Study is one of the largest studies of this kind major results are expected. The ethical issues involved in this study were already taken care of by the study organizers and pose no risk for griddification



Genetics (HTS-Analysis)

HTS-Analysis: High-Throughput Sequencing is a pipeline analysing the data coming from high-throughput sequencers. The 5-10 Terabytes originating from the sequencer comes split in relatively tiny pieces and has to be formatted, processed and mapped to a reference sequence. This is done in mainly 3 steps consisting of i) image analysis, ii) individual "shot-gun" sequence determination, and iii) assembly of the entire genomic sequence. The functioning of this pipeline is proven and is used in daily work. Due to the importance of high-throughput sequencing for research and diagnostics, this is a prime application for grid with major impact. All ethical issues in terms of data privacy were already taken care of by the providers of the material and pose no risk for griddification.

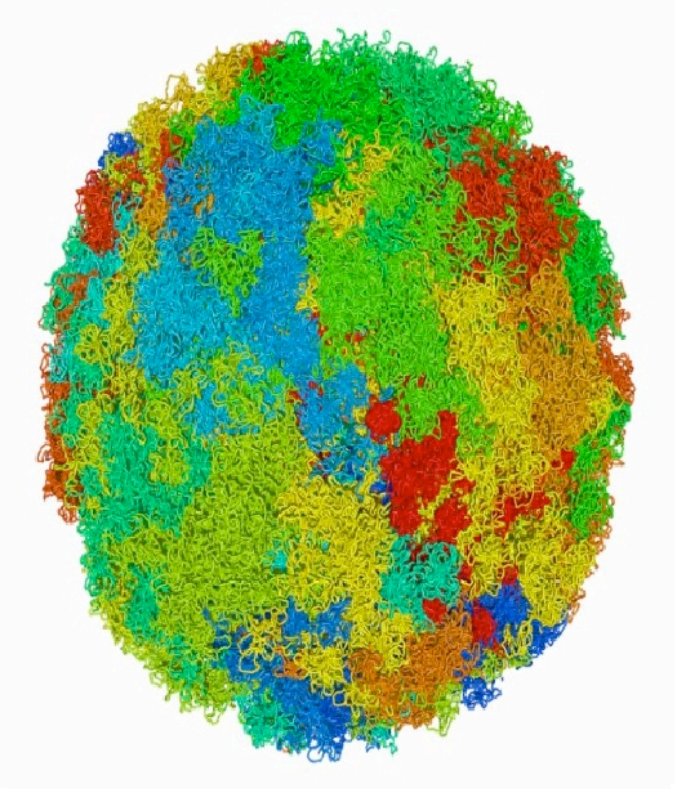


Genetics (DNA-ORG)

DNA-ORG: The major task in genomics is sequence comparison and pattern recognition within this sequence. DNA-ORG consists of three major and new algorithms to i) make exact comparisons between sequences, ii) find arbitrary patterns in genetic sequences, and iii) localized patters in sequences. Currently, DNA-ORG is used to analyse these parameters in ~8,000 completely sequenced genomes with a high impact for the understanding of genomes. Beyond, with the just starting boom in HTS there are unprecedented opportunities for grid based high-performance computing. All ethical issues in terms of data privacy were already taken care of by the providers of the material and pose no risk for griddification.

VirtNuc

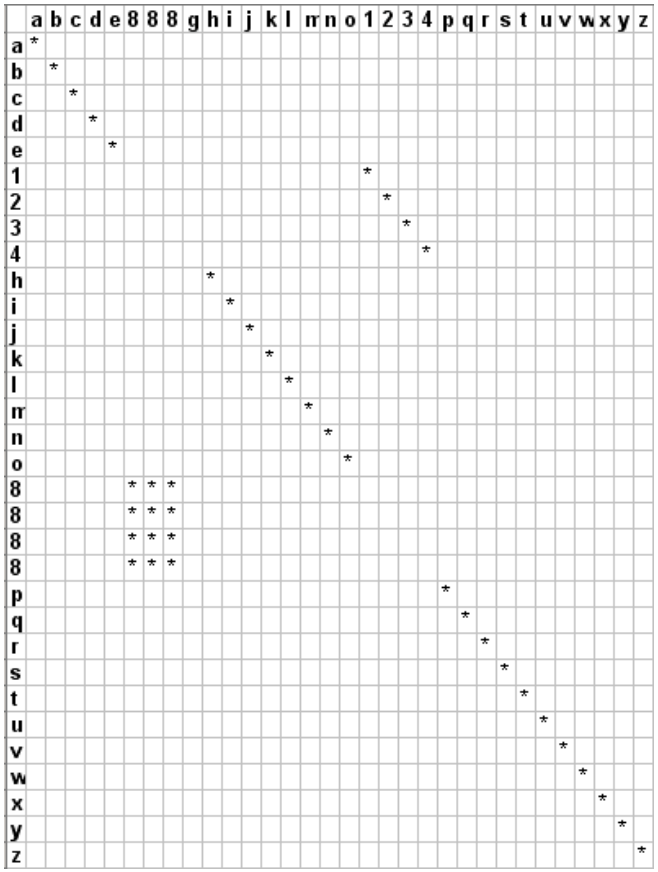
VirtNuc: The application VirtNuc which makes simulations of large macromolecular polymer structures. It is able to simulate extremely large structures. Currently, it is used to predict the archtictural/3D organization of the human genome by simulating all chromosomes in the cell nucleus assuming the chromatin fibre as consisting of 2,400,000 million segments. With Monte-Carlo and Brownian Dynamics methods configurations of chromosomal topologies and the entire mitosis, i.e. nuclear cell-cycle are simulated and used for prediction and comparison to experiments. This is of major importance for genetic understanding, diagnostics and treatment in the framework of genetic engineering for disease treatment. No ethical issues what so ever apply.



Alignment Algorithms

	Time	Space
Needleman-Wunsch-Gotoh	$\mathcal{O}(N^2)$	$\mathcal{O}(N^2)$
Smith-Waterman-Gotoh	$\mathcal{O}(N^2)$	$\mathcal{O}(N^2)$
Hirschberg-Myers-Miller	$\mathcal{O}(N^2)$	$\mathcal{O}(N)$
variant Needleman-Wunsch-Gotoh	$\mathcal{O}(N^2)$	$\mathcal{O}(\max(N, L^2))$
variant Hirschberg-Myers-Miller	$\mathcal{O}(N^2)$	$\mathcal{O}(N)$

Dot plot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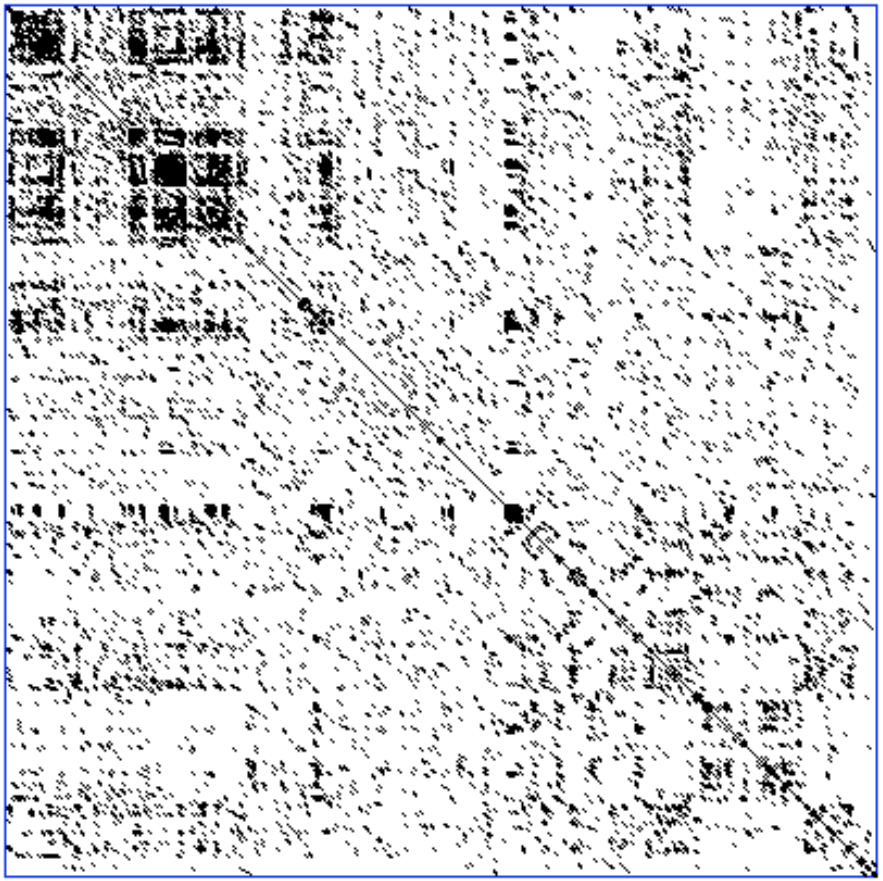
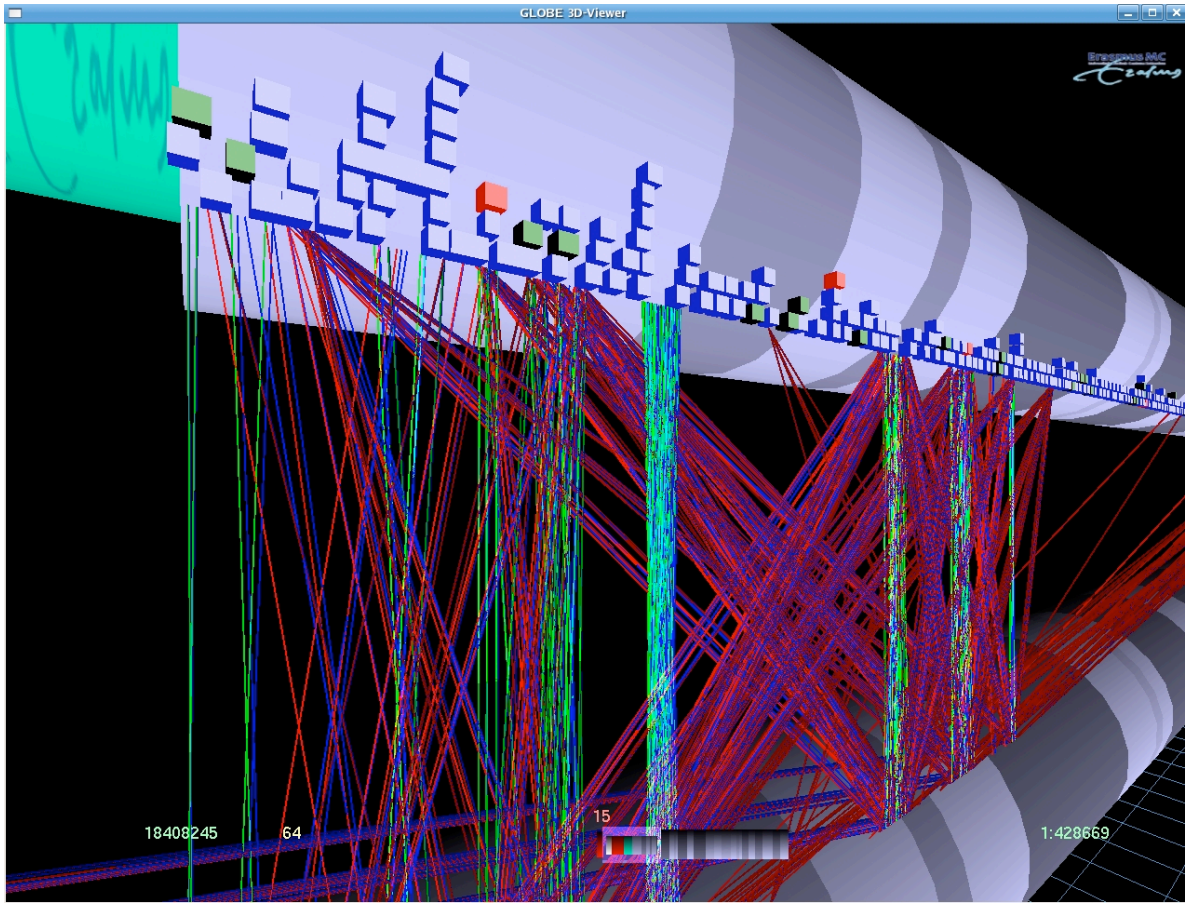


Visualization of Results in DNA viewer



Prader-Willi syndroom


Questions?

Porting Biomedical Applications to Grids

Knoch, T. A.

1st EDGeS grid training workshop & 2nd AlmereGRID grid experience workshop. Almere, The Netherlands, 27th - 29th November, 2008.

Abstract

Today advances in scientific research as well as clinical diagnostics and treatment are inevitably connected with information solutions concerning computation power and information storage. The needs for information technology are enormous and are in many cases the limiting factor for new scientific results or clinical diagnostics and treatment. At the Hogeschool Rotterdam and the Erasmus MC there is a massive need for computation power on a scale of 10,000 to 15,000 computers equivalent to ~20 to ~30 Tflops (10^{12} floating point operations per second) for a variety of work areas ranging from e.g. MRI and CT scan and microscopic image anlysis to DNA sequence analysis, protein and other structural simulations and analysis. Both institutions have already 13,000 computers, i.e. ~18 Tflops of computer power, available!

To make the needed computer power accessible, we started to build the Erasmus Computing Grid (ECG), which is connecting local computers in each institution via central management systems. The system guaranties security and any privacy rules through the used software as well as through our set-up and a NAN and ISO certification process being under way. Similar systems run already world-wide on entire institutions including secured environments like government institutions or banks. Currently, the ECG has a computational power of ~5 Tflops and is one of or already the largest desktop grid in the world. At the Hogeschool Rotterdam meanwhile all computers were included in the ECG. Currently, 10 departments with ~15 projects at the Erasmus MC depend on using the ECG and are preparing or prepared their analysis programs or are already in production state. The Erasmus Computing Grid office and an advisory and control board were set-up.

To sustain the ECG now further infrastructure measures have to be taken. Central hardware and specialist personal needs to be put in place for capacity, security and usability reasons for the application at Erasmus MC. This is also necessary in respect to NAN and ISO certification towards diagnostic and commercial ECG use, for which there is great need and potential. Beyond the link to the Dutch BigGrid Initiative and the German MediGRID should be prepared for and realized due to the great interest for cooperation. There is also big political interest from the government to relieve the pressure on computational needs in The Netherlands and to strengthen the Dutch position in the field of high performance computing. In both fields the ECG should be brought into a leading position by establishing the Erasmus MC a centre of excellence for high-performance computing in the medical field in respect to Europe and world-wide.

Consequently, we successfully started to build a super-computer at the Hogeschool Rotterdam and Erasmus MC with great opportunities for scientific research, clinical diagnostics and research as well as student training. This will put both institutions in the position to play a major world-wide role in high-performance computing. This will open entire new possibilities for both institutions in terms of recognition and new funding possibilities and is of major importance for The Netherlands and the EU.

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Keywords:

Genome, genomics, genome organization, genome architecture, structural sequencing, architectural sequencing, systems genomics, coevolution, holistic genetics, genome mechanics, genome function, genetics, gene regulation, replication, transcription, repair, homologous recombination, simultaneous co-transfection, cell division, mitosis, metaphase, interphase, cell nucleus, nuclear structure, nuclear organization, chromatin density distribution, nuclear morphology, chromosome territories, subchromosomal domains, chromatin loop aggregates, chromatin rosettes, chromatin loops, chromatin fibre, chromatin density, persistence length, spatial distance measurement, histones, H1.0, H2A, H2B, H3, H4, mH2A1.2, DNA sequence, complete sequenced genomes, molecular transport, obstructed diffusion, anomalous diffusion, percolation, long-range correlations, fractal analysis, scaling analysis, exact yard-stick dimension, box-counting dimension, lacunarity dimension, local nuclear dimension, nuclear diffuseness, parallel super computing, grid computing, volunteer computing, Brownian Dynamics, Monte Carlo, fluorescence in situ hybridization, confocal laser scanning microscopy, fluorescence correlation spectroscopy, super resolution microscopy, spatial precision distance microscopy, auto-fluorescent proteins, CFP, GFP, YFP, DsRed, fusion protein, in vivo labelling, information browser, visual data base access, holistic viewing system, integrative data management, extreme visualization, three-dimensional virtual environment, virtual paper tool.

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