

# The VASP Software GmbH: Why did we go commercial?

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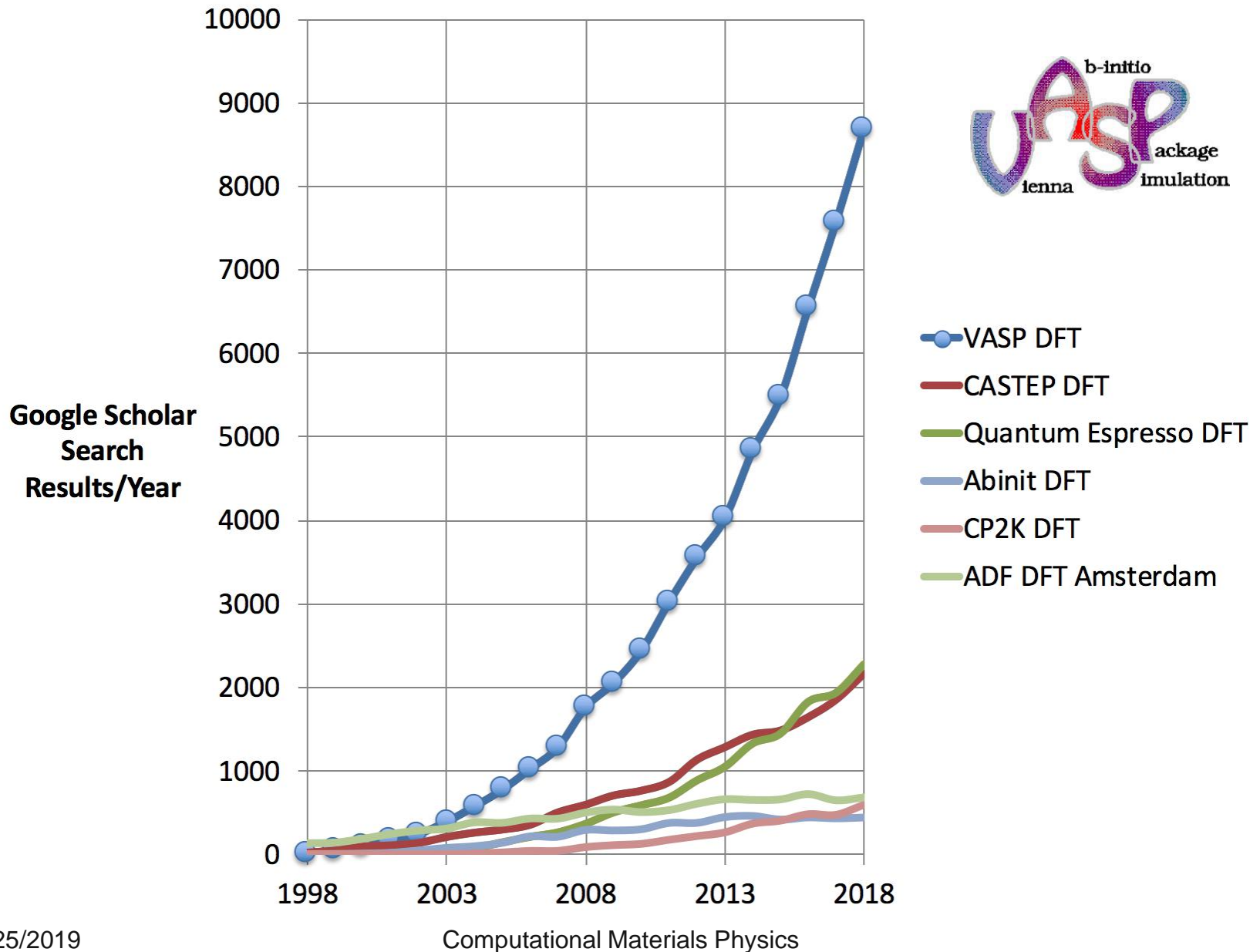


# Background information on VASP

- VASP: Vienna ab initio Simulation Package
- Electronic structure code
  - Kohn-Sham density functional theory
  - Many body Schrödinger equation using diagrammatic techniques
- For solids, the most widely used code right now
  - Estimated user base between 5.000-15.000 users (personnel cost: 1 Billion/year)
- VASP: Little to no GUI and/ or workflow management
- Hybrid licensing model: proprietary but source code distributed



# VASP impact (Google scholar citation analysis)



- Off the shelf **pseudopotentials for all elements** in the periodic table since 20 years
  - G Kresse, D Joubert, PRB 59, 1758 (1996)
    - Single control instance generating and updating the potentials
    - Users can be certain to use the best possible compromise between efficiency and robustness
- **Unprecedented robustness** since 20 years
  - G. Kresse, J. Furthmüller, PRB 54, 11169 (1996)
    - Charge density mixing, which was against the main stream Car-Parrinello idea in 1996
    - Sufficiently robust for high throughput screening
- **State of the art**: hybrid functionals, beyond DFT

# Some lessons I have learned over the years

- Electronic structure theory
  - Requires a great expertise typically 1-3 years into the PhD people are capable to contribute to the code  
for DFT 1-2 year, diagrammatic methods 2-3 years
- Less than 1 % of the practitioners examine and study the codes (fairly tiny developer basis)
- “The cathedral and the bazaar” (Eric S. Raymond, 1997)
  - Cathedral: code developed between releases is restricted to an exclusive group of software developers
  - Bazaar: code is developed over the Internet in view of the public



# Successful electronic structure codes

- Tend to lean towards the **cathedral model**
  - There is an exclusive group controlling
    - The pseudopotentials
    - What goes into main stream code
    - What should be added and rewritten
- Cathedral model applies to VASP
  - Combined with my knack for engineering,  
→ very robust and fast code

# The code complexity

- Most electronic structure codes are large and complex
- VASP approaches now  
500.000 lines of Fortran 90 legacy code
  - This is small compared to other e.g. quantum chemistry codes
  - Although one does not need to understand the entire code in order to contribute, **steep learning curve**
  - Documentation is not great, because personnel to do this was (and is still) lacking
  - **Effort for refactoring, rewriting and documentation is most likely on the order of 50 men years in the next 10 years or 5 million Euro!**
- No funding agency is ever going to fund this effort

# Funding situation

- Funding in particular in the US is predominantly for **engineering**, but hardly ever for development or coding
- In the EU this situation is slightly better
- However, a proposal only has chances of success, if it **progresses sciences**
- **Code refactoring and rewriting is not funded**  
This means that codes become potentially more complex, less clear and less well maintained over time
- **Support is not funded**  
Experts become quickly overwhelmed by support

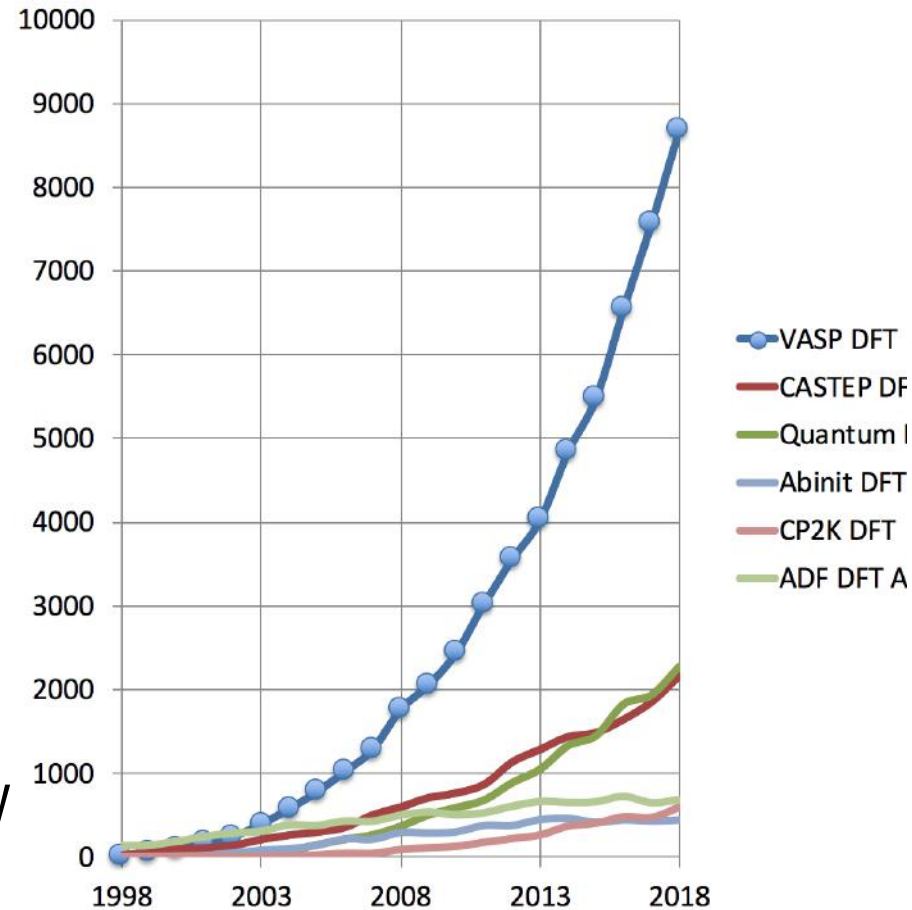


# Typical approach in Science

- **Misuse funding received for fundamental research**
  - Receive funding for fresh idea
  - PhD PostDocs spend initial time in documenting existing legacy code
  - Only very slow progress in actual functionality
- Funding for governmental or non-profit entities to write new codes from scratch
  - Hardly ever successful, but there are exceptions (LAMMPS)
- **Infrastructure funding by the EU**

# Infrastructure funding by the EU

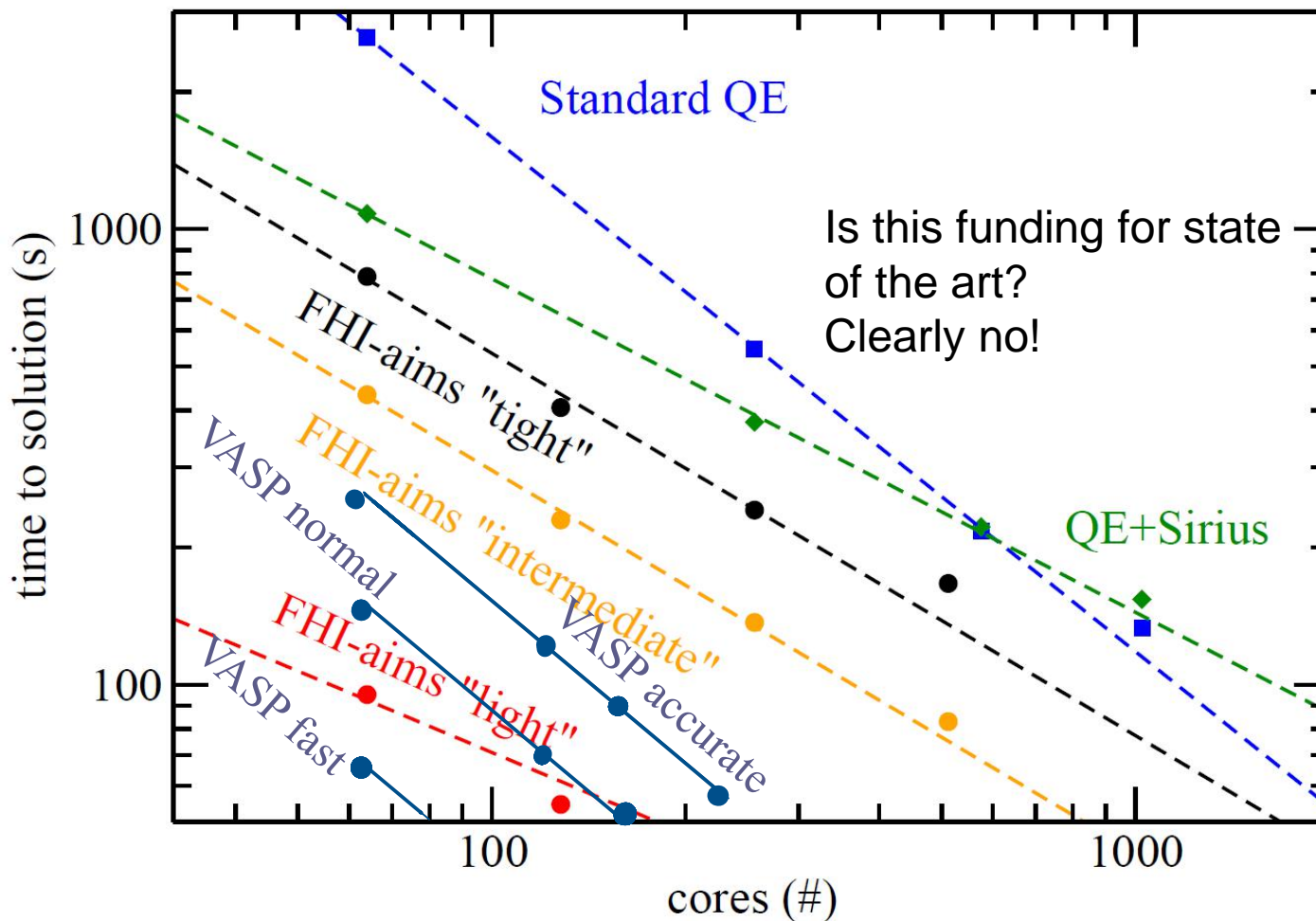
- ETSF  
European theoretical spectroscopy  
Facility
- Psi-k
- Exascale initiative of the EU
  - MaX Centre of excellence  
Quantum Espresso, Yambo,  
Siesta
  - NOMAD and NOMAD-XT  
FHI-AIMS, VASP, abinit, GPAW
  - One was funded  
I doubt the money will be  
used for refactoring



# Infrastructure funding by the EU

QE+ Sirius: Sirius a software library for PW codes (MaX):  $\text{SiO}_2$

QE <https://www.quantum-espresso.org/news-events/news/2167/Kozhevnikov.pdf>



# Let the users decided not the referees

- Infrastructure funding of software is difficult
  - Funding agency need to rely on expert referee reports
  - Referees tend to credit writing skills, international connections, novelty and not user base and user needs
- Why not adopt the best practice model: market
  - Let the market/user decide which code they want to use!
  - Involves a license fee
- Counterargument against commercialization:
  - Funding was originally by public hand
  - However, this is only a fraction of the total software cost

# Funding of scientific software

- Cutting edge developments & novelty:
  - Funded by national funding agencies and EU
  - In development projects, the actual investment into coding is small, on the order of 20-30 % of the total time
  - 70-80 % into scientific exploration/ paper writing/ testing
- Exploitation and marketing of developed ideas must be considered a bonus
  - Code rewriting, refactoring
  - Careful documentation
  - Ease of use and automatization
  - Support

# VASP the hybrid marketing model

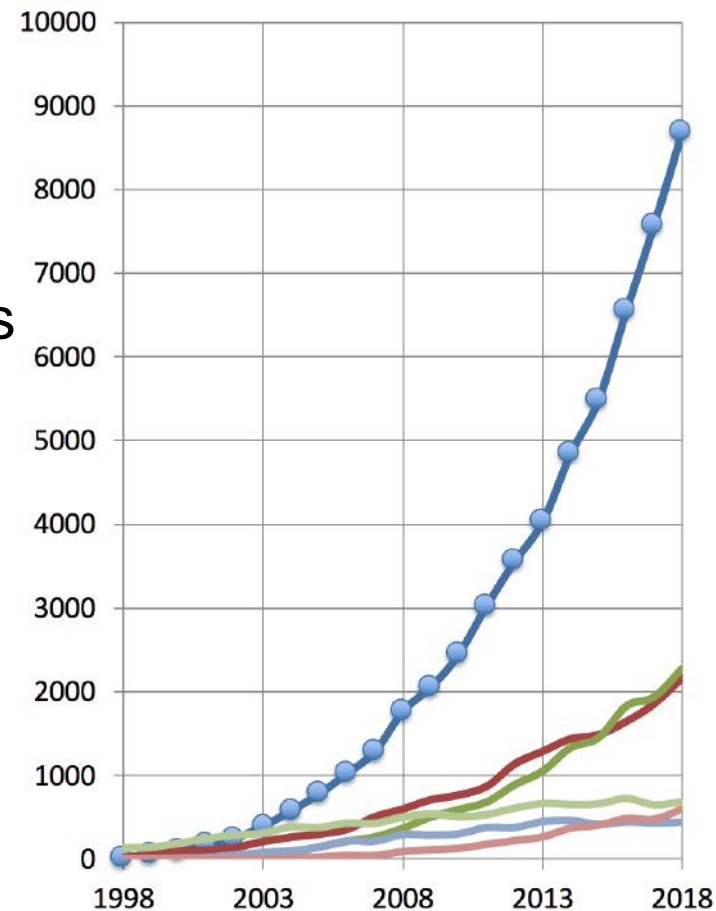
- VASP until 2018 developed at the University of Vienna
  - Supervised mostly by myself (and Martijn Marsman)
  - Typical academic fee **4000,- Euro** for a permanent **source code** license without upgrades/ updates or support
  - Based on trust and registered users
  - Complimentary user forum and email support
  - Affordable fee given that the personnel cost is about 60.000-120.000,- Euro per year
  - Too cheap, but there are open source alternatives!
- This model was conceived by Jürgen Hafner
  - Akin to typical quantum chemistry models
  - Robust revenue stream in the last 20 years



# VASP biggest hurdles

Long time commitment of University is on shaky grounds

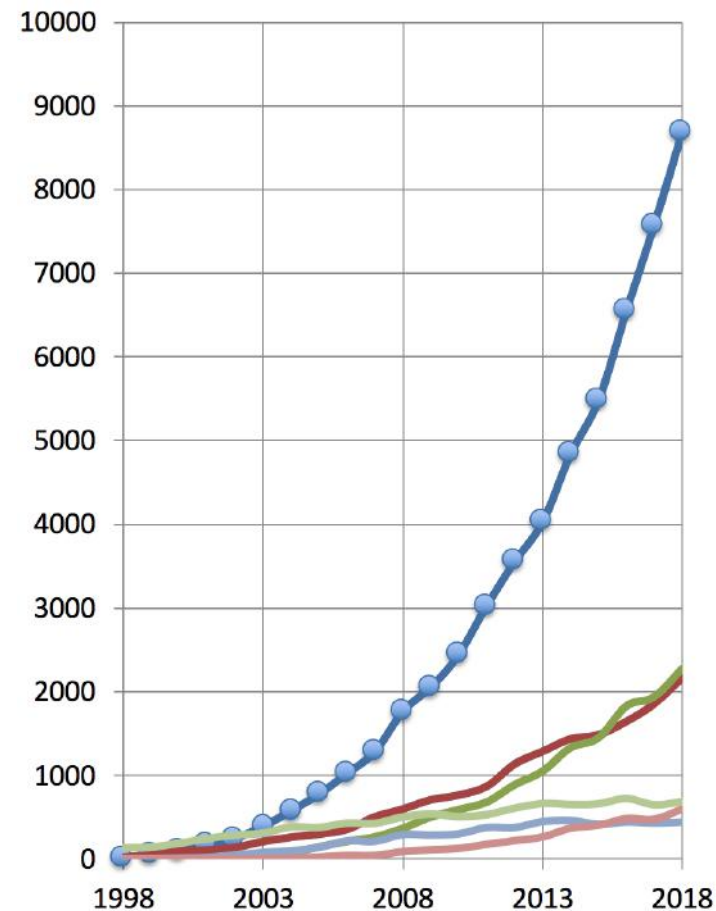
- 2017: three permanent employees
- Employees became progressively overwhelmed by work
- Other contracts strictly limited to 6 years  
3-4 years PhD  
2 additional years for PostDoc  
Most PostDocs left earlier
- As explained above, first principles codes are complex and require 2-4 years of expertise



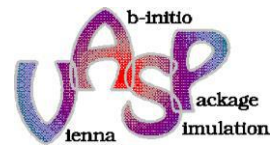
# VASP biggest hurdles

Long time commitment of University is on shaky grounds

- Relationship depends on Rectorate  
current relationship is superb  
but might change at any time
- What happens beyond my own  
involvement with VASP?
- Code is not going away,  
on the contrary user basis grows!
- Only long time solution is an  
independent company



- Founded September 2018
- Jointly owned by University of Vienna, Georg Kresse and team members
- Main goals: robustness, documentation, support, ...
- Novel developments
- License model remains unchanged
  - Direct marketing of **source code** to academia for VASP.6 for a **modest fee**
  - Commitment to 3 years upgrades and updates
  - Marketing to industry through (lack of GUI)



# VASP the team



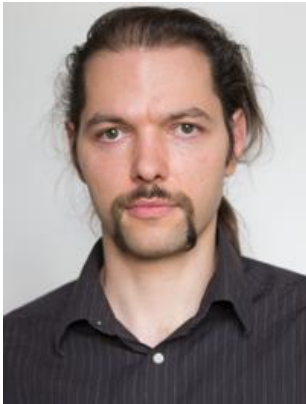
Georg Kresse



Martijn Marsman



Doris Vogtenhuber



Ferenc Karsai



Merzuk Kaltak



Marin Schlipf

And continuing to hire

One issue I encountered:

VASP users often have little expertise in code development

Recruiting mainly previous open source developers!

# Some Conclusions

## ● *Funding*

- Possible for cutting edge developments but not refactoring, documentation, support (sustainability)

## ● *Progressing the field*

- Mostly academia, a strong case for open source
- Commercial exploitation is required

## ● *Barriers*

- The European physics community believes in open source
- Not sustainable, I believe
- Good software is never free or cheap

## ● *Usage of codes*

- Large user basis in academia: in total 10.000+ users
- Industry certainly behind like 10 years