

The VASP Software GmbH: Why did we go commercial?

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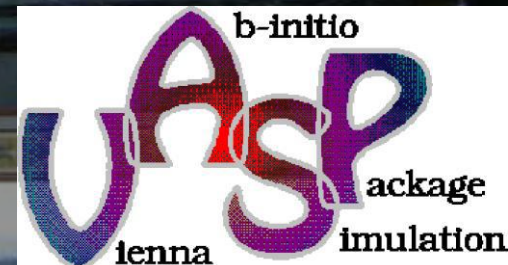
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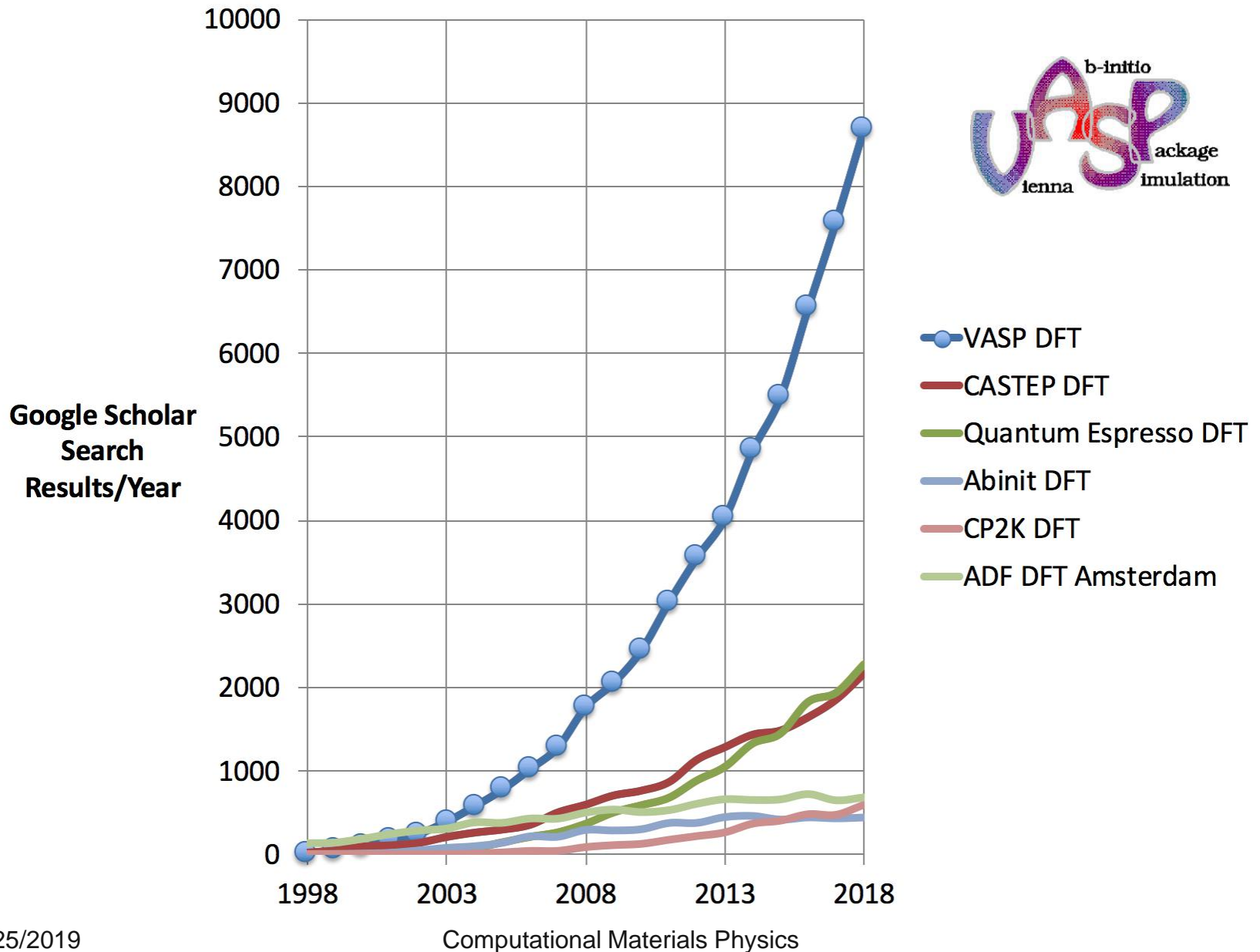


Background information on VASP

- 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

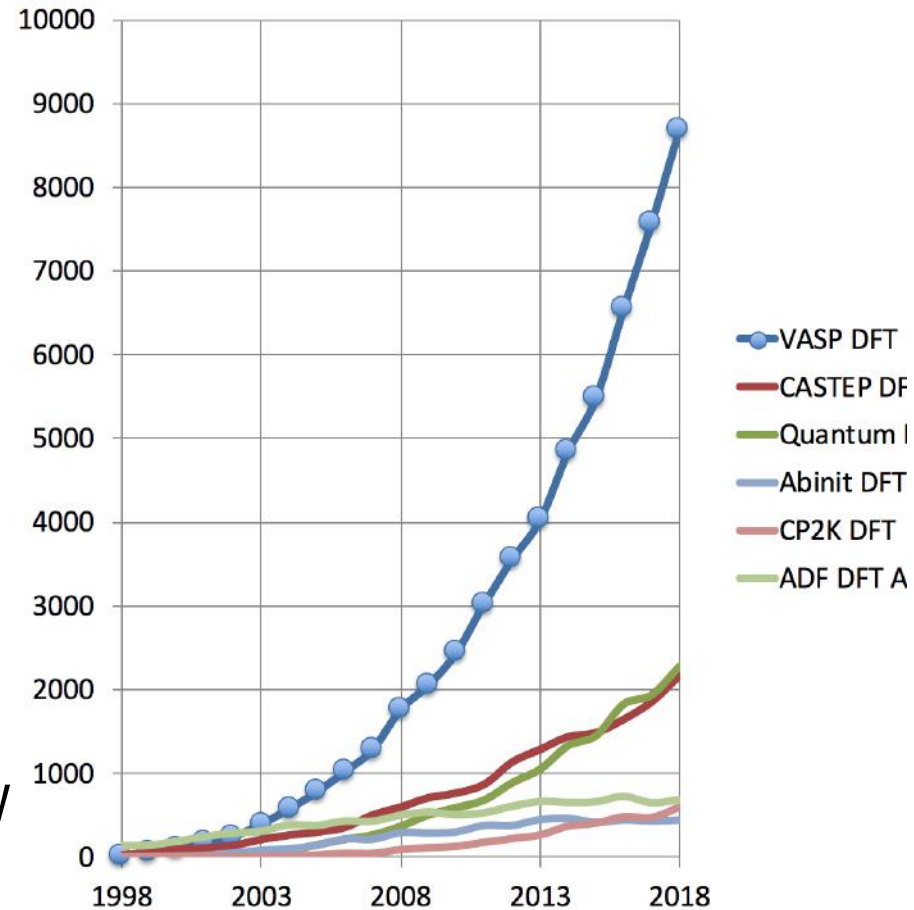
- Funding in particular in the US is predominantly for **engineering**, but hardly ever for development or coding
- In the EU this situation is slightly better
- However, a proposal only has chances of success, if it **progresses sciences**
- **Code refactoring and rewriting is not funded**
This means 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

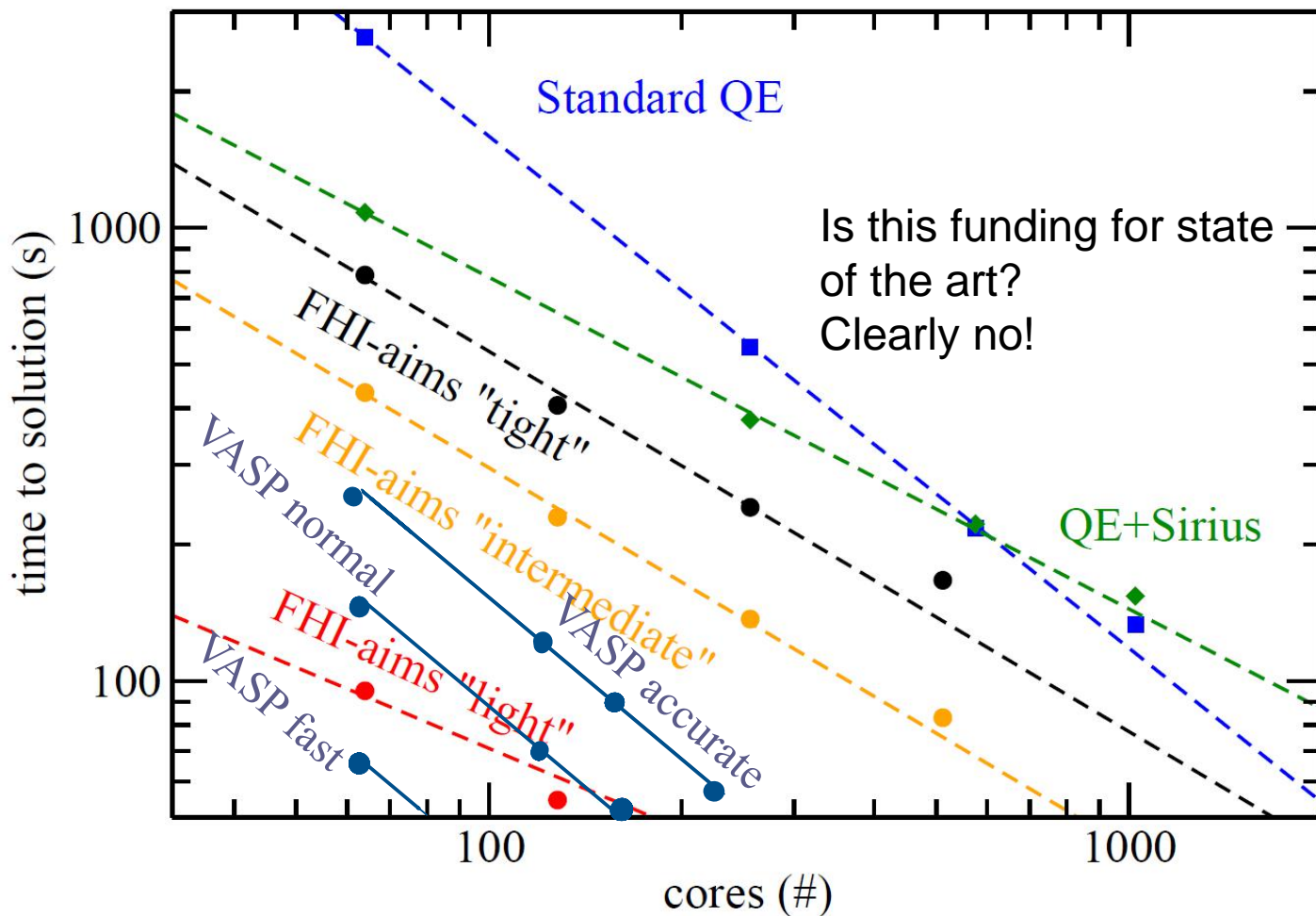
- ETSF
European theoretical spectroscopy
Facility
- Psi-k
- Exascale initiative of the EU
 - MaX Centre of excellence
Quantum Espresso, Yambo,
Siesta
 - NOMAD and NOMAD-XT
FHI-AIMS, VASP, abinit, GPAW
 - One was funded
I doubt the money will be
used for refactoring



Infrastructure funding by the EU

QE+ Sirius: Sirius a software library for PW codes (MaX): 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

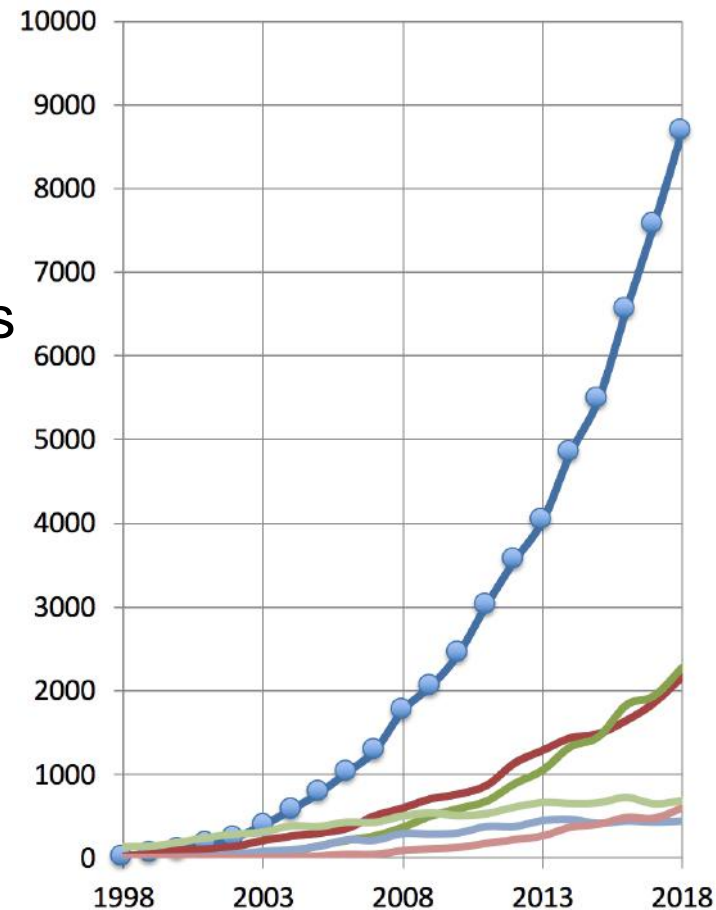
VASP the hybrid marketing model

- 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

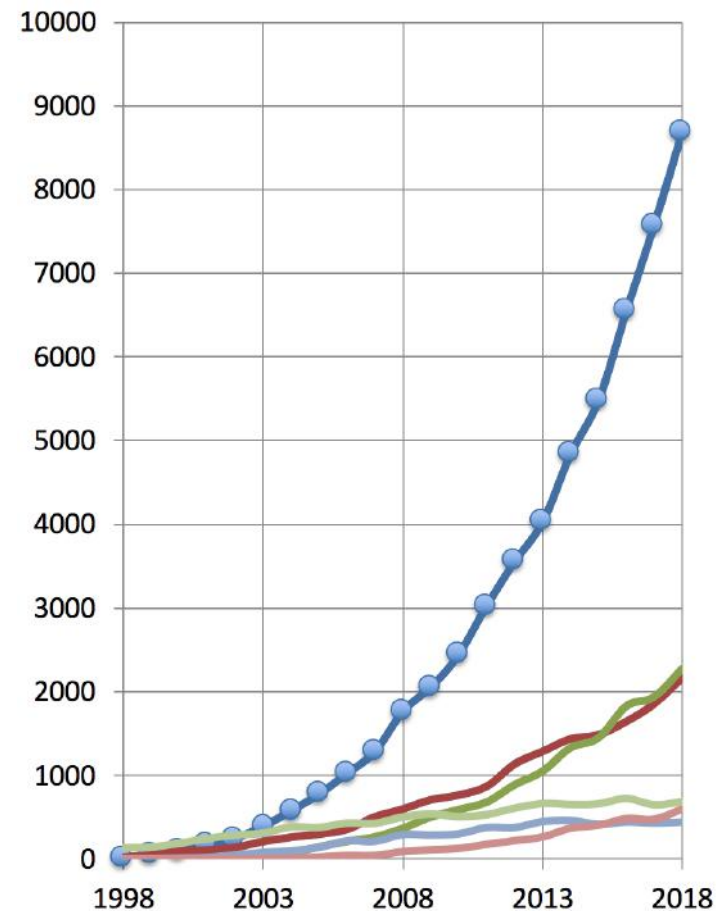
- 2017: three permanent employees
- Employees became progressively overwhelmed by work
- Other contracts strictly limited to 6 years
3-4 years PhD
2 additional years for PostDoc
Most PostDocs left earlier
- As explained above, first principles codes are complex and require 2-4 years of expertise



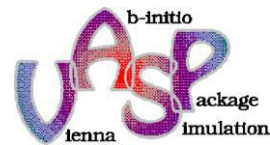
VASP biggest hurdles

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



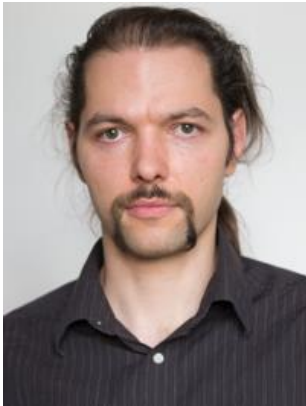
Georg Kresse



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