



The European Materials Modelling Council

# Meeting of the EMMC

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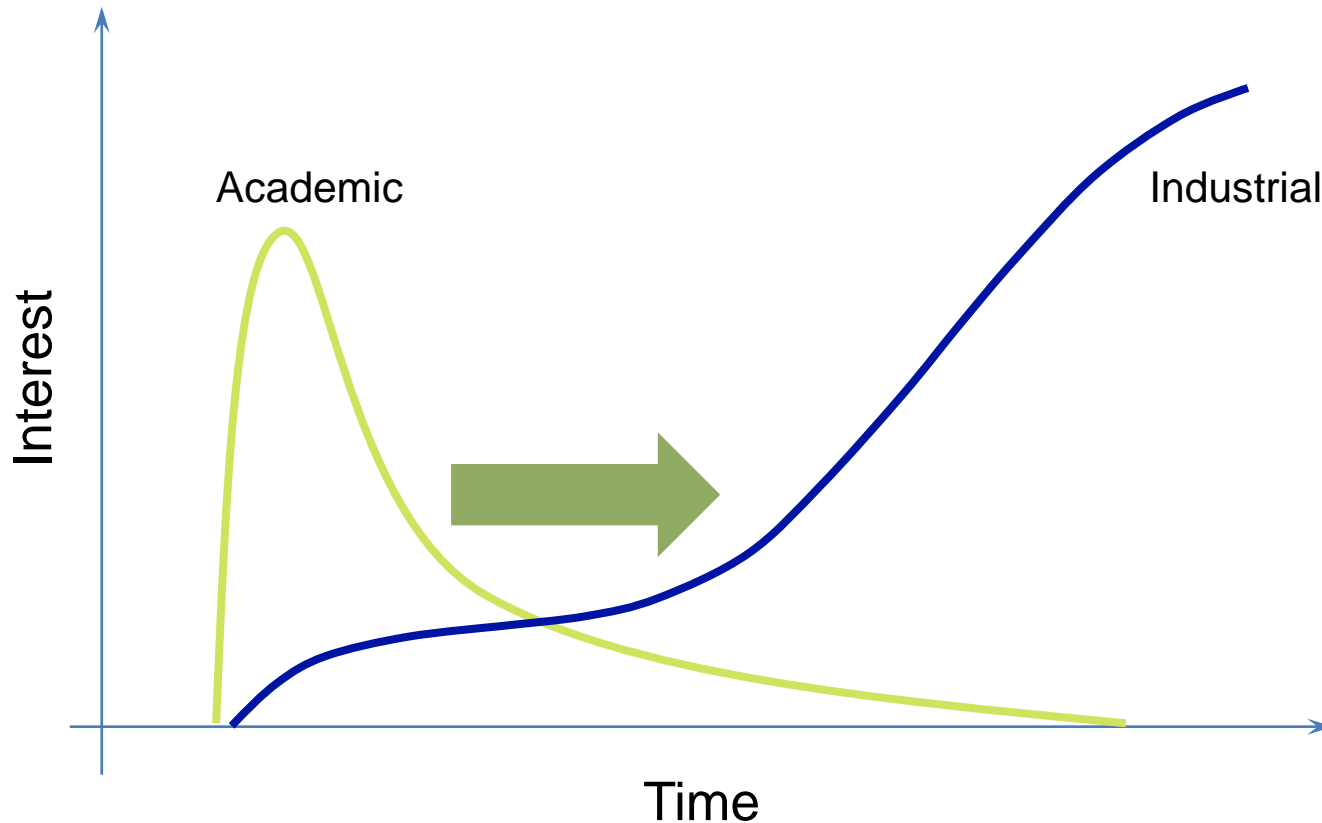
## Recommendations for Academic Materials Modelling Software Engineering



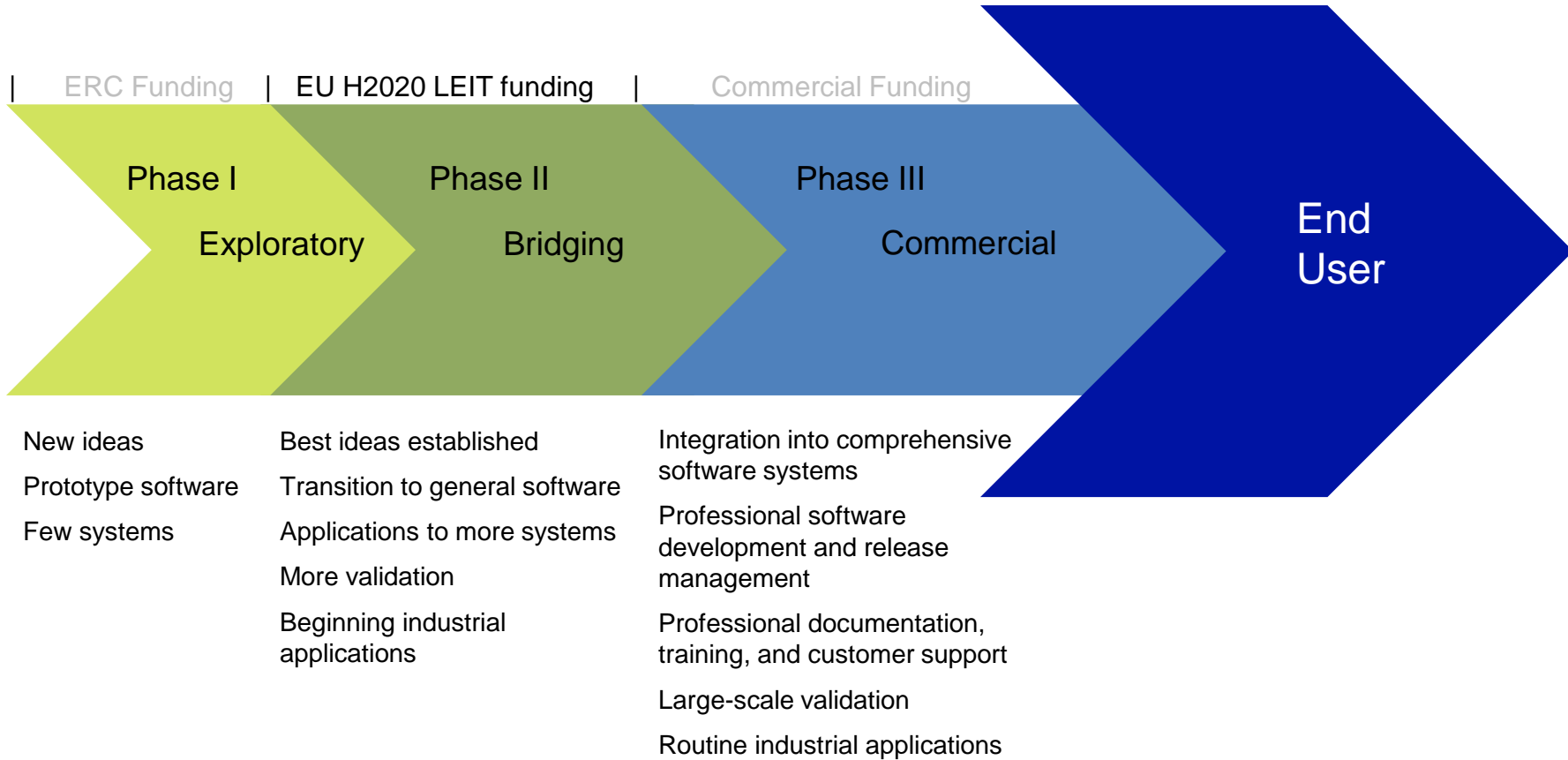
# Outline

- ▶ Phases of Software
- ▶ Interests of SWO's
- ▶ Software Quality
- ▶ Recommendations
- ▶ Licencing
- ▶ Summary

# Phases of Software Technology



# Phases of Software Development und Use





# Phase II

## ▶ Phase II a

- Generalisation of software
- Proof of concept
- Collaboration between industrial scientists and software developers

## ▶ Phase II b

- Solution of particular problems of industrial relevance
- Validation



# Interest of SWO

- ▶ Integration of models and codes covering full range of length and time scales from electronic to macroscopic levels
- ▶ Growing industrial use of computational materials engineering
  - Communication with and education of the market
  - Enable also SME's to benefit from this software technology
- ▶ Development of modelling community and networking
- ▶ Standardisation
- ▶ Validation and references
- ▶ Support from High Performance Computing facilities

See also: "Materials Modelling: Where do we want to go?", Edited by A. F. de Baas (2014)



# Software Quality

## Requirements by SWO's

- ▶ Understand
  - ▶ Adapt (integrate, connect)
  - ▶ Enhance
  - ▶ Maintain
- 
- Code design
  - Stability and resilience
  - Modularity
  - Performance



# Proposed Recommendations

1. Document functionality and accuracy in academic publications
2. Provide wider applicability via validation on a set of fully documented test cases; use specific industrial examples
3. Demonstrate good numerical implementation and numerical stability; use software metrics
4. Provide complete documentation including the connection of underlying equations with code variables; choice of algorithms; manuals and tutorials
5. Include test procedures and document test results
6. Document code versions used for specific tests
7. Document IT requirements (operating system, compilers, MPI, etc.)
8. Consider the integrability of the new “content blocks” into existing “mainstream software”
9. Demonstrate interest of potential end-users
10. Consider the type of end-use, i.e. broad applicability vs. high-value niche applications
11. Adopt a licence model allowing commercial industrial use
12. Collaborate with SWO in the entire process





# Licencing

## ► Information for developers on licence schemes

- GPL: “viral”, tends to block commercial use – not recommended
- LGPL – better than GPL, but still poses problems for SWO’s
- BSD, Apache – permissive in using code as building blocks in integrated software systems
- Dual licencing – distinguish between academic and commercial licences
- One-to-one licencing



# Regulatory

- ▶ Virtual testing and modelling considered in norms and regulations



# Summary

- ▶ Three phases of software development
  - Focus on Phase II (“Bridge Phase”)
- ▶ Interest of SWO’s
  - Providing integrated and supported software solutions in a sustainable and economically viable business model
- ▶ Software Quality
  - Working with academic software developers to enable successful transfer of their codes or “content blocks” into industrial use
- ▶ Recommendations
  - 12 recommendations including licencing