EMMC-Webinar
on
Best Practices for Software Development

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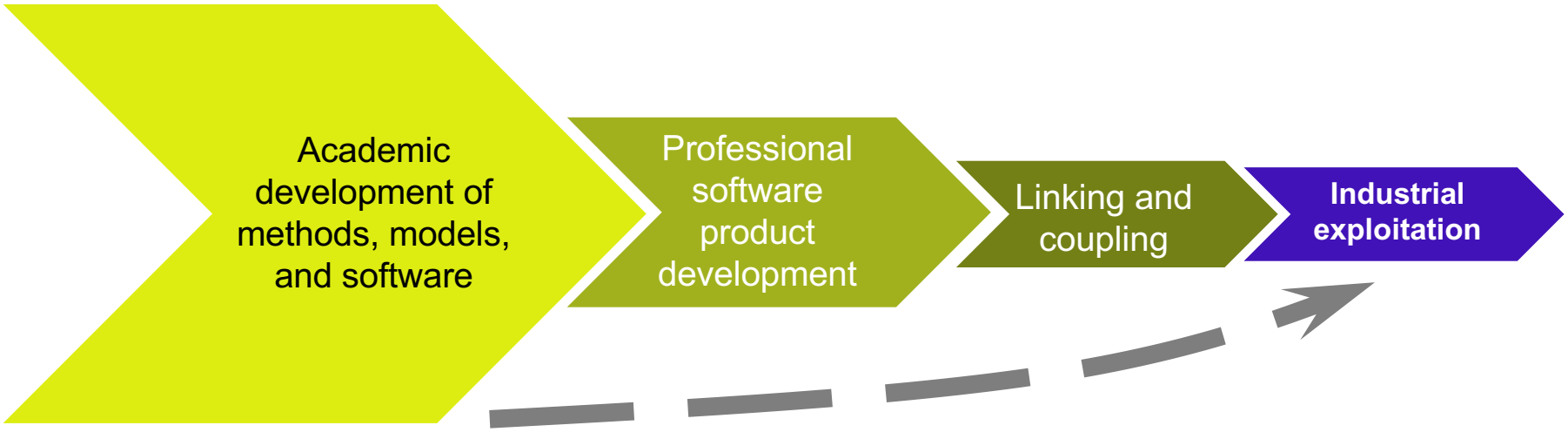
Agenda

- Introduction
- Scope
- Model description and software architecture
- Programming language and deployment
- Intellectual property and license considerations
- Testing, verification, validadation and robustness
- Organization of software development
- Version control
- Metadata
- Documentation
- Support
- Conclusion

Current Deployment of Academic Software



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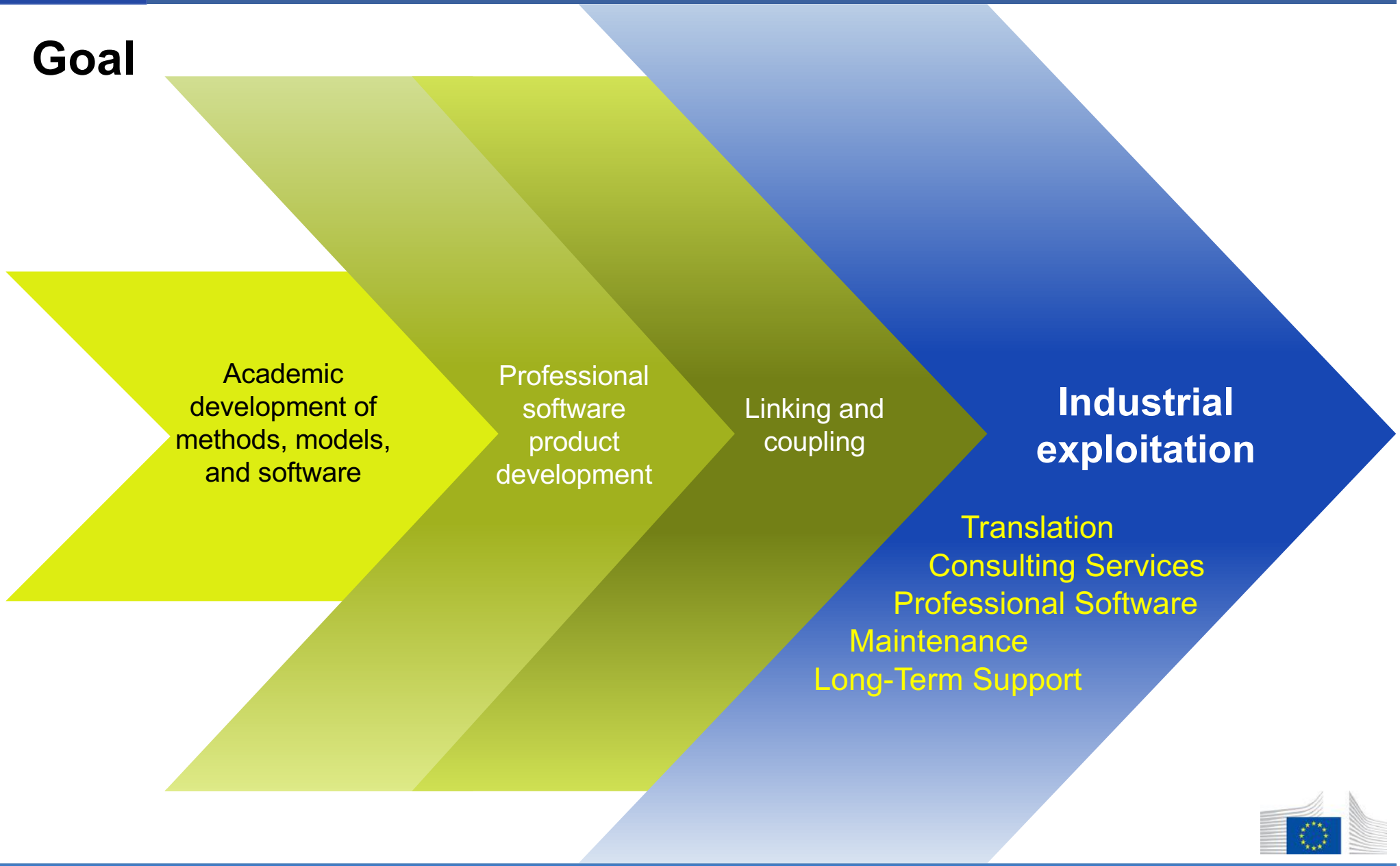
Industrial Software Deployment

Goal



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Introduction

- EMMC-CSA (Coordination and Support Action):
  - Installed in 2016 by European Commission
  - Foster materials research in European industry
  - Stimulate materials modelling as integral part of industrial R&D
  - Combines expertise of academic and industrial partners
  - Strengthen link between (academic) software developers, distributors, and (industrial) end users
- White paper/webinar on software development:
  - Provide academic researchers with guidelines for sustainable modelling-software development
  - Increase awareness of importance of early design decisions
  - Share best practices of software development

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Scope

- Huge amounts of scientific software developed over decades:
  - Mainly in academia, mainly by students and postdocs (who soon after left), short time horizon
  - Often “Quick and dirty” coding, lack of documentation
  - Less emphasis on IP and licensing considerations
- Increasing degree of commercialization:
  - Quantum chemistry codes → chemical and pharmaceutical industry
  - Companies like Biovia (Biosym, MSI, Accelrys), Materials Design, Schrödinger, QuantumWise/Synopsys, SCM establishing value-added chain from academic research to industrial deployment
- Software-development guidelines for academic developers
  - More rapid integration of academic software with industrial software

Model Description and Software Architecture

- Early planning:
  - Scope of the software
  - Vision for future developments
- Software Architecture:
  - Modularization, well-defined interfaces
  - Use libraries (*e.g.* LAPACK) whenever possible
  - Try to combine selected software modules into a library that can be shared and maintained by several groups (*e.g.* libxc)

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Programming Language and Deployment

- Fortran (I-IV, 66, 77, 90, 95, 2003, 2008, 2018):
  - Probably most used language in scientific computing
  - Tremendous move from “spaghetti code” to modern object-orientation
  - Upward-compatibility saves investment in decades of code development
  - Good performance, many compilers available (free and commercial)
- C++:
  - Object oriented, requires some computer science skills to master
  - Increasingly used for scientific applications
  - Good performance, compilers available
- Python:
  - Increasingly popular in scientific community
  - Interpreter, fast prototyping, less performant, errors to be found at run time
  - Can be interfaced with compiled language at increased complexity

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Programming Language and Deployment

- Parallel programming:
  - MPI
  - OpenMP
- GPU programming:
  - CUDA
  - OpenACC
- Coding guidelines
  - Increase readability and improve work in a development team
  - Try to use community standards and be consistent
- Source-code documentation
  - At the disposal of single developer but strongly (!) recommended
  - Can/should be done according to rules defined by development team
  - Allows for automatic documentation through Doxygen or Sphinx

Intellectual Property and License Considerations

- Legal matters:
  - not exciting to deal with but utterly important
  - decisions at an early stage of crucial importance, especially when many people are involved
- Ownership:
  - employer or employee?
- Intellectual property rights:
  - copyright, patent?
  - national laws, international regulations?
- License models:
  - permissive, copyleft, proprietary?

Intellectual Property and License Considerations

Permissive licenses, free and open-source software (FOSS):

- Free software (Free Software Foundation, 1986):
  - Freedom 0: The freedom to **run** the program for any purpose
  - Freedom 1: The freedom to **study** how the program works, and change it to make it do what you wish
  - Freedom 2: The freedom to **redistribute** and make copies so you can help your neighbour.
  - Freedom 3: The freedom to **improve** the program, and release your improvements (and modified versions in general) to the public, so that the whole community benefits
- Open Source Definition (Open Source Initiative, 1998):
  - Based on Debian Free Software Guidelines
  - Largely equivalent
- others: Berkeley Software Distribution, MIT, Apache, Educational Community License

Intellectual Property and License Considerations

Copyleft licenses:

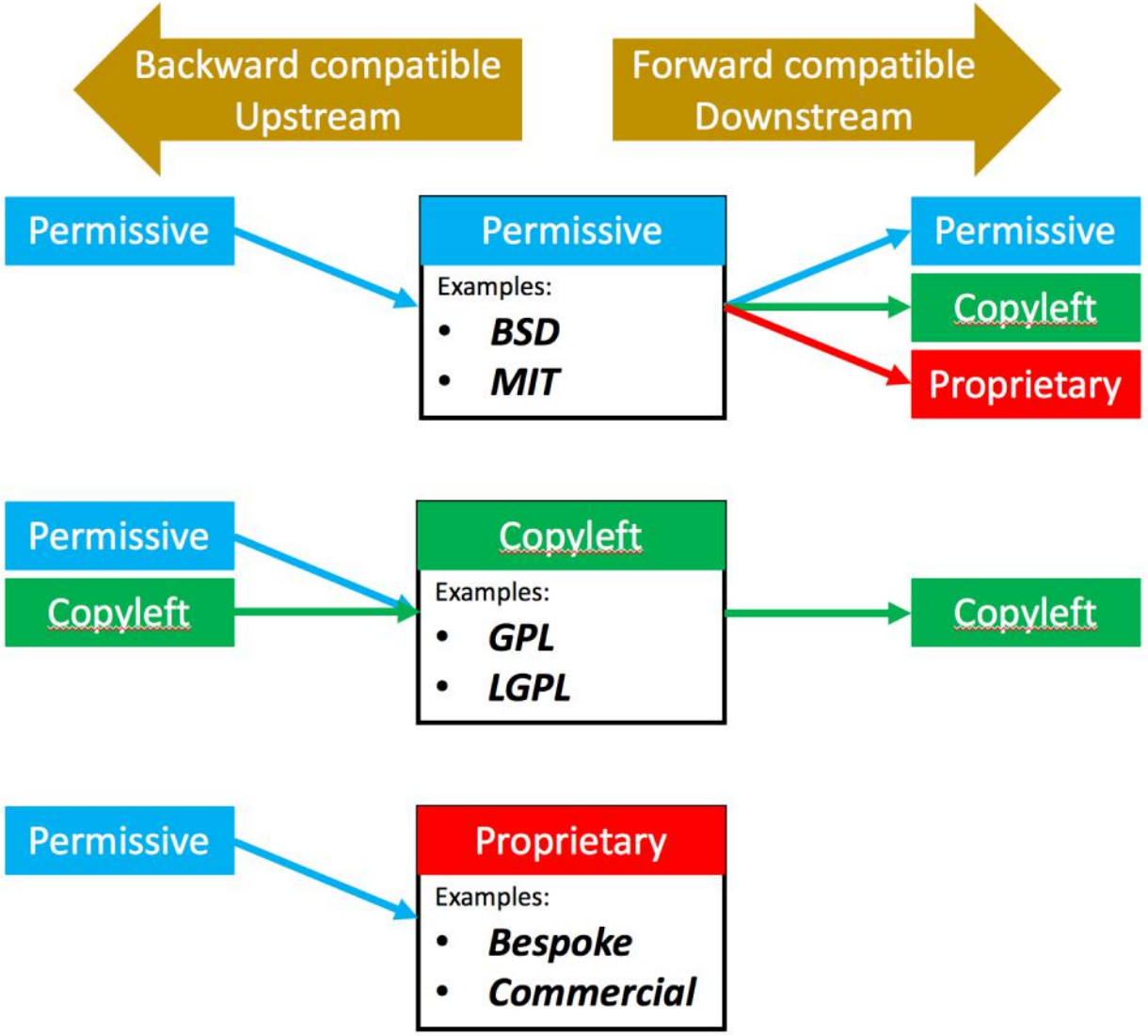
- apply to free and open source software
- modified versions must preserve freedom 0-3 (viral licenses)
- examples
  - GNU General Public License (GPL)
  - GNU Lesser General Public License (LGPL)
  - Mozilla Public License (MPL)

Proprietary licenses:

- include constraints (no source code, license fee)
- often come with commercially developed software
- often come together with long-term support

Intellectual Property and License Considerations

License schemes
- Combination
- Directionality



A. Morin *et al.*, PLoS Comp. Biol. **8**, e1002598 (2012)

Intellectual Property and License Considerations

Copyright and licensing in practice: first steps

- Add Copyright line to each file
  - Version MyCode 29.05.2018 MyFirstName MyLastName
  - Copyright © 2018 MyFirstName MyLastName
  - Please see file MyCopyrightFile for details.
- Create a MyCopyrightFile
  - Include GPL/LGPL as available from gnu.org
  - Alternatively include BSD, MIT, … license files available from the respective sources

Testing, Verification, Validation, and Robustness

- Testing:
  - Includes all parts of a software
  - Considers different platforms (hardware architectures, operating systems)
  - Ensures consistency of results obtained from different releases
  - Ideally done at a hierarchy of time intervals and complexities
- Verification:
  - Compare with other implementations or with prototypes of less complexity
- Validation:
  - Comparison of calculated results to experimental data
- Robustness:
  - Make sure that the implementation does not only work for simple test systems

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Organization of Software Development

- Scrum model:
  - Iterative development by a team of developers in short development cycles (sprints), typically 3-week cycles

Phases:

- Planning
- Sprint
- Demo
- Retrospective

Version Control

- Version control systems:
  - Record all changes to the code
  - Archive and allow recovery of all previous states of the code
  - Coordinate parallel editing of the same piece of code by several developers
  - Allow simultaneous work on different branches of the code
  - Allow merging different branches of the code
  - Centralized vs. distributed systems
- Basic functionality of VCS:
  - Check out from central repository to local working directory of developer (copy/lock vs. copy/merge systems)
  - Local work of developer
  - Check in to central repository (with time stamp and user ID)
  - Synchronization with other developers work

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Metadata

- Much underrated and rarely considered
- Crucially important and prerequisite for reproducing results
- Should include
  - Version/release number/release date
  - Copyright and licensing information
  - development group/developer
  - Compiler and compiler options
  - Hardware used to run a calculation
  - User running the calculations and working directory
  - Start and end time of calculations
  - Complete list of all input data
  - all information in all intermediate/output files (check internal consistency)

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Documentation

- Model description
- Design guidelines (code architecture, accuracy, limitations)
- Technical documentation of implementation using, e.g., sphinx or doxygen
- User documentation (user's guide)
- Video tutorials
- Marketing (raise initial interest, address decision makers)

User Documentation

- Installation guide: first contact, clear, mention auxiliary software
- Case studies and workable examples
- Complete list of all variables (default values, physical units, criticality, sensitivity of results to changes)
- Complete list of all input/intermediate/output files (role, size)
- Graphical user interface (screenshots)
- Background information on
  - Model description and algorithms
  - Software architecture and implementation
  - Limitation
  - Selected input parameters

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Support

Support at its best

- Long-term stability
- Long-term maintenance (updates, enhancements)
- Hotline, 24h response
- Connect to industrial software owners

Conclusion

- Early design decisions are mandatory:
  - Scope of software, vision of future development
  - Model description, software architecture, programming language
  - Organization of software development process
  - License model (proprietary, permissive, copyleft)
  - Version control, source-code documentation
  - Testing, verification, and validation
  - User documentation and support

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