

E-CAM

Supporting HPC Simulation in Industry and Academia

09 May 2016 | Alan O'Cais
E-CAM Software Manager

a.ocais@fz-juelich.de

What is E-CAM?

- An e-infrastructure for software, training and consultancy in simulation and modelling
- A partnership of
 - 16 CECAM nodes
 - 3 PRACE Centres
 - 12 Industrial Partners
 - 1 Centre for Industrial Computing
- 5 year time frame

Areas of Expertise

- CECAM
 - Domain and scientific expertise
 - Organisational
- PRACE partners
 - Application porting and benchmarking
 - Training expertise
 - HPC system knowledge

Who are our users?

- CECAM family of computational science researchers
 - Pan-European distributed network of scientists and research centres
 - computational simulation techniques at the atomic, molecular and increasingly at the supra-molecular level
 - physics, chemistry and the life sciences
- In industry we have a significant community of scientists who are using these same techniques to address problems of direct relevance to industry
 - 12 industrial partners part of project

What are our applications?

- No particular applications chosen in advance
 - User driven selection – „State of the Art“ workshops
 - Pilot research projects with industry
- Applications are mainly in the classical domains of:
 - quantum dynamics
 - electronic structure
 - molecular dynamics
 - mesoscale simulations

Libraries

- Application Library
 - Usage information
 - Build recipes
 - Regression tests and benchmarks
- Software Library
 - Develop new or refactor existing code
 - Extract transferable components
 - Create language wrappers
 - Use best practices (documentation, unit tests, regression tests, code review,...)

(Web) Services

- (Automated) Style Guides
- Build system template/advice/support
- Continuous Integration framework
- Documentation framework
- Collaborative tools (EtherPad, ShareLatex)
- Support of applications for PRACE resources
- Version control (GitHub/GitLab)
- Onboarding support
- Training Portal

Training

- Diverse target audience requires diverse training
- Many people are (potential) HPC users but not necessarily potential HPC developers
 - Need to support core skill sets for effective resource use
 - Provide development path
 - Collaboratively created content for common skills
- Targeted training at appropriate level for audience
 - Leverage PRACE training events for specialised training
 - Leverage CECAM for scientific training and collaboration

Working towards Exa-scale

- Current focus on accessing and exploiting existing resources
 - Expand the community
 - Promote best practices for software development
- WP7: „Hardware considerations and the PRACE relationship”
 - filtering layer for the complex hardware initiatives
 - identify knowledge gaps before they hinder progress
 - translate into recommendations for targeted training initiatives

Extended Software Development Workshops

- 2 week training and code development event
- Scientific components
 - Methods, applications and algorithms
 - Establishing goals
- Technical components
 - Software development best practices
 - Documentation, performance analysis,...
 - Exposure to new tools/technologies
- Build catalogue of vertical/horizontal training material

Relationship with industry

- Enable software that can be more easily adopted by industry
- Consulting role (open to academia and industry)
 - From 'easy': What method/application to choose?
 - To hard: implement new methods, solve a particular problem
- Initially 12 industrial partners (with seed projects)
- Industry part of governance structure
- Sustainability depends on mutually beneficial relationship with industry

Collaborations and Synergies

- Training
 - PRACE
 - Other COEs
 - SC: „Best Practices in HPC Training“
 - Software Carpentry ('HPC Carpentry')
- Best practices for software development
- Application developers

Comments and Questions

