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**Q1** What is your organisation's/project's name?

E-CAM Centre of Excellence

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**Q2** Your organisation's/project's website

<https://www.e-cam2020.eu/>

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**Q3** Are you?

**A project**

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**Q4** Your name

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**Q5** Your email address

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**Q6** Your contact phone number

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**Q7** Please summarise who you are and what you do

The E-CAM Centre of Excellence supports HPC simulations in industry and academia through software development, training and discussion in simulation and modeling. E-CAM is based around the experience and scientific community of the extended CECAM family, established over more than four decades and central in promoting fundamental research on advanced computational methods, as well as the computational and hardware expertise of the European partnership PRACE. We are a partnership of 16 CECAM Nodes, 3 PRACE centres, 13 industrial partners and one Centre for Industrial Computing (the Hartree Centre at Daresbury). Our training and software development activities are spread across Europe at the different Node locations.

E-CAM is funded by the European Union Horizon 2020 research and innovation program; has a 60 month duration (October 2015 - September 2020) and involves 48 staff years of effort. The coordination of E-CAM is located at the École polytechnique fédérale de Lausanne, in Switzerland.

Our approach is focused on four scientific areas, critical for high-performance simulations relevant to key societal and industrial challenges. These areas are classical molecular dynamics, electronic structure calculations, quantum dynamics and meso- and multi-scale modelling. E-CAM develops new scientific ideas and transfers them to algorithm development, optimisation, and parallelization in these four respective areas, and delivers the related training. Postdoctoral researchers are employed under each scientific area, working closely with the scientific programmers to create, oversee and implement the different software codes, in collaboration with our industrial partners.

The goals of E-CAM are to:

- Develop software modules to be used in academia and industry to solve simulation and modelling problems; and to interface those software modules with standard codes and tune the outputs to run on the next generation of exascale computers;
- Create an open-access E-CAM Software Repository containing robust applications, modules, scripts, and wrappers, for simulations in material science, life science and engineering; and set software standards through best practice guidelines to ensure that appropriate documentation and metadata supports the use of the software;
- Provide information and opportunities for discussion on leading-edge simulation and modelling techniques. This includes workshops with industry to identify areas of mutual interest as well as the development of on-line training resources. We have strong industry links with eight industry pilot projects running since the start of the project;
- Train the next generation of computational scientists from both industry (new managers and computing specialists) and academia (post-graduates and postdocs); and ensuring that there are continuing professional development opportunities for scientists and that our links with industry will provide career progression for the participants of our workshops.

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**Q8** In what way would like to contribute to an EsD project? **As a HPC user** ,  
**An an application provider**

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**Q9** What would be your contribution to an EsD project?

- High throughput computing applications targeting the materials sciences community
  - Two applications that are members of the High-Q club Jülich [http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/\\_node.html](http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/_node.html) - IMD and MP2C
  - Access to the E-CAM user community and the associated training infrastructure
  - Software installation framework (Easybuild)
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**Q10** What partners are you looking for?

- Technology providers
  - System integrators
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**Q11** Please include links to any additional material.

<https://www.e-cam2020.eu/>

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**Q12** Other comments/ideas

**Respondent skipped this question**

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