

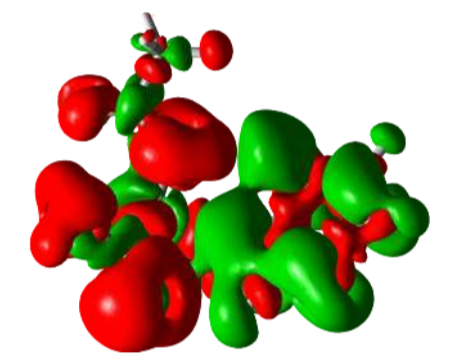
[www.e-cam2020.eu](http://www.e-cam2020.eu)



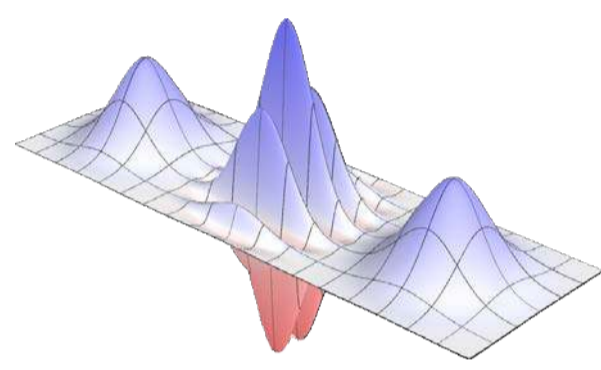
## European Centre of Excellence

for software development, training and industrial discussion in simulation and modelling

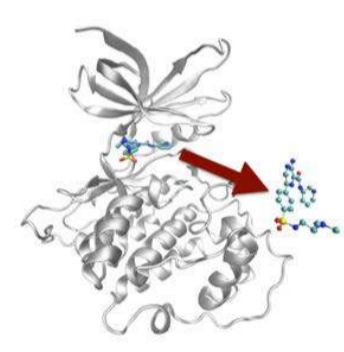
### OUR SCIENTIFIC AREAS



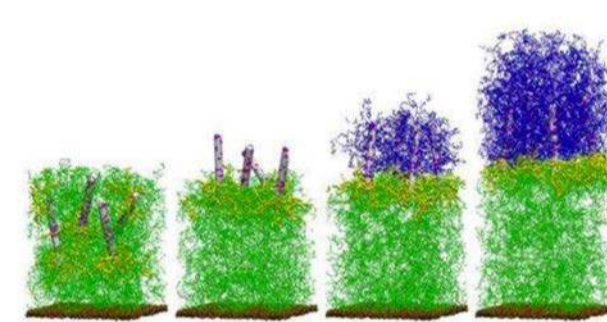
Electronic Structure



Quantum Molecular Dynamics



Classical Molecular Dynamics



Mesoscale Modelling

### OUR SERVICES

#### SOFTWARE DEVELOPMENT



**Modular software** to be used in academia and industry to solve simulation and modelling problems. **Development of transversal tools** to improve performance and scalability, with potential for benefiting a large community.

#### TRAINING



**Train scientists from industry and academia** on the development of methods and software scaling towards the high end of HPC systems through **extended software development workshops** and **industry training events**.

#### CONSULTANCY

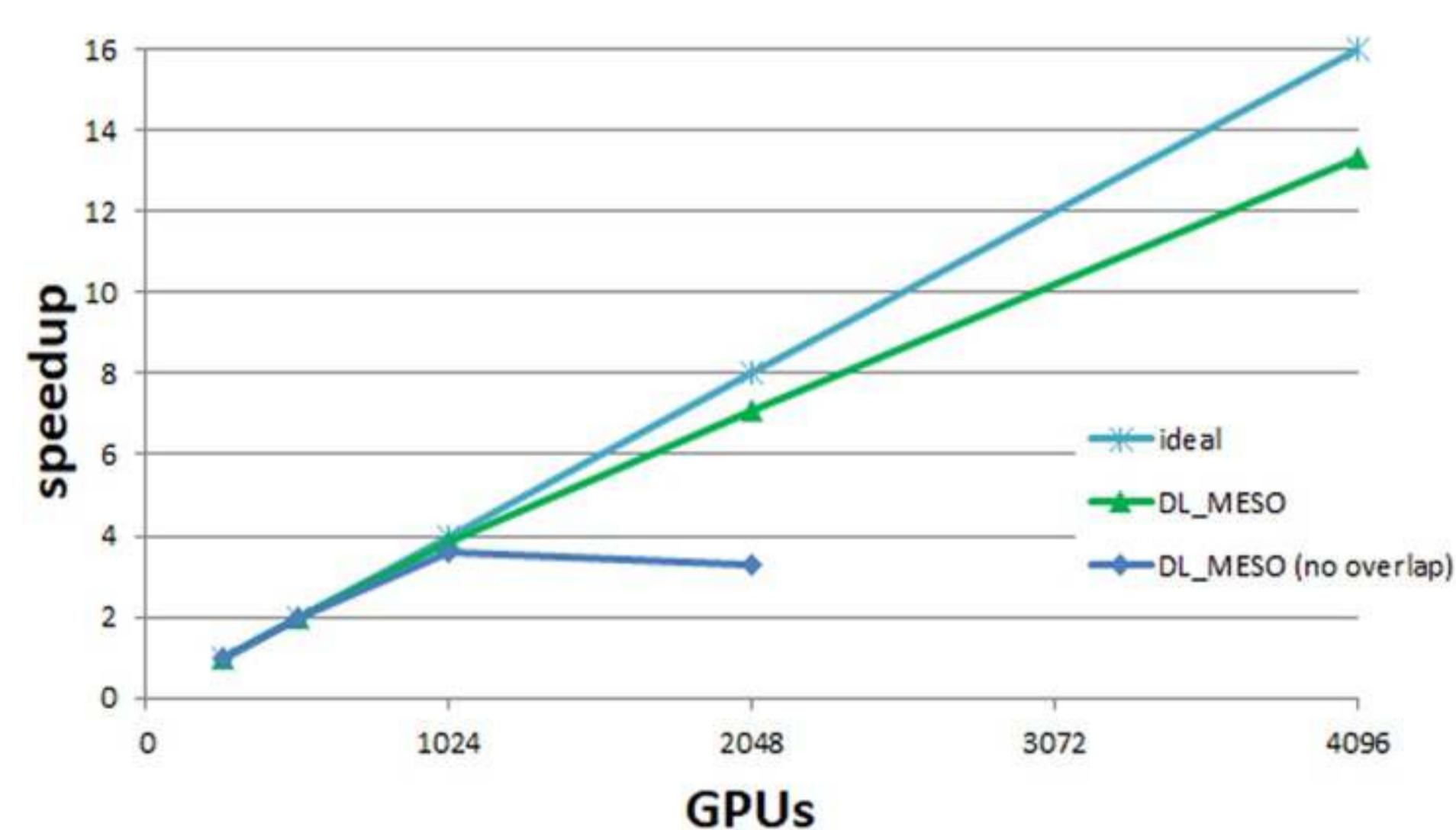


Provide **opportunities for discussion** on leading-edge simulation and modelling techniques. This includes workshops with industry to identify areas of mutual interest as well as the possibility to engage in **direct discussions with experts in the CECAM community**.

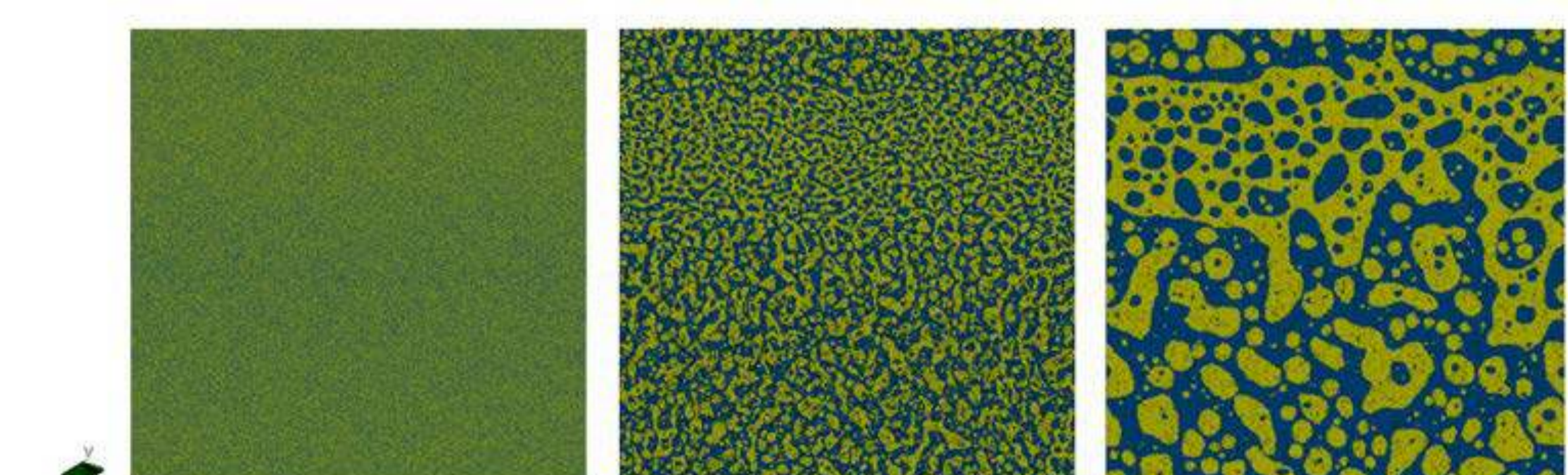
### USE CASE

*Mesoscale simulation of billion atom complex systems using thousands of GPGPUS's*

- E-CAM has developed a highly efficient version of DL\_MESO (DPD), a software package for mesoscale simulations developed at the UKRI STFC.
- This distributed GPU acceleration development is an extension of the DL\_MESO package to MPI+CUDA that exploits the computational power of the latest NVIDIA cards on hybrid CPU-GPU architectures.
- The need to port DL\_MESO to massively parallel computing platforms arose because often real systems (e.g. surfactants, which are key ingredients in personal care products, dish soaps, laundry detergents, etc) are made of millions of particles and small clusters are usually not sufficient to obtain realistic results in brief time.
- DL\_MESO is used for a wide range of problems of both scientific and industrial interest.



*DL\_MESO\_GPU strong scaling up to 4096 GPUs. This allows the simulation of very large systems like a phase mixture with 1.8 billion particles (below).*



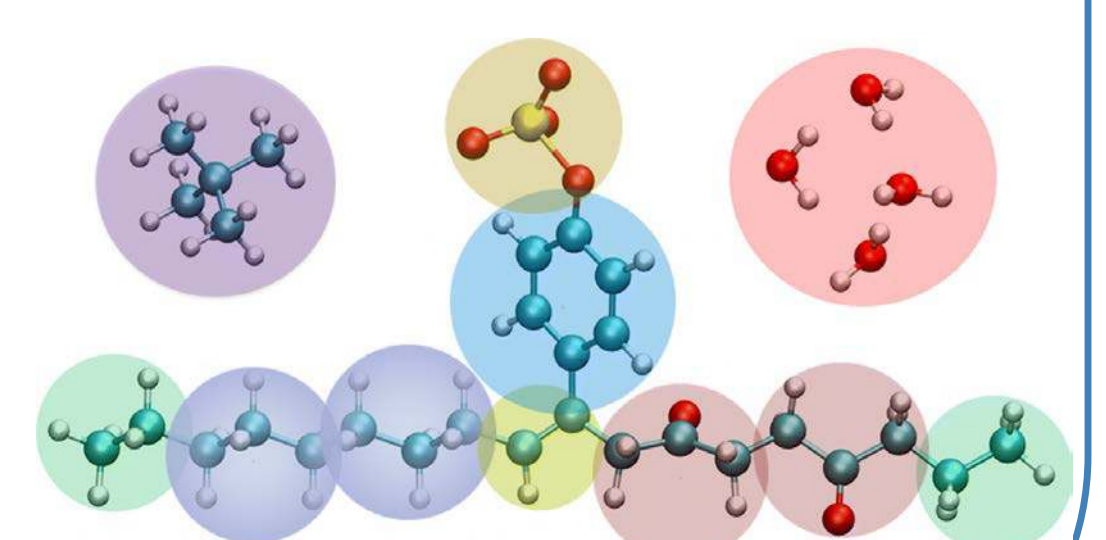
*Time evolution of a binary phase separation for a system made up of 1.8 billion particles, on the GPU version of DL\_MESO.*

#### Industry training at the MESOSCALE

22 - 25 March 2021 - ONLINE

*Training event dedicated to INDUSTRY, on Dissipative Particle Dynamics simulations and the use of DL\_MESO\_DPD*

[www.cecama.org/workshop-details/1074/](http://www.cecama.org/workshop-details/1074/)



E-CAM is coordinated by [CECAM](http://www.cecama.org). It is a partnership of 16 CECAM Nodes, 2 PRACE centers and 1 center for Industrial Computing (Hartree Centre).



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