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## CRESTA and the exascale challenge

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With thanks to Professor Mark Parsons for relevant slides

The University of Edinburgh

## Collaborative Research into Exascale Systemware, Tools and Applications - CRESTA

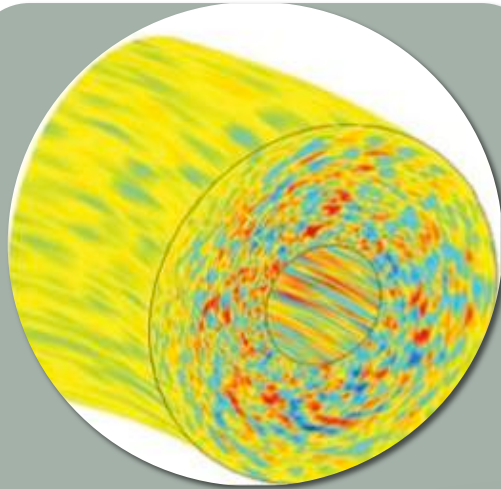
- Exascale Software
- 3 years - €100M
- Leading European research centres
  - EPCC – Edinburgh, UK
  - HLRS – Stuttgart, Germany
  - CSC – Espoo, Finland
  - KTH – Stockholm, Sweden
- A world leading vendor
  - Cray UK – Reading, UK
- World leading tools providers
  - Technische Universitaet Dresden (Vampir) – Dresden, Germany
  - Allinea Ltd (DDT) – Warwick, UK
- University College London – UK
- ECMWF – Reading, UK
- Ecole Central Paris – Paris, France
- DLR – Cologne, Germany
- KTH – Stockholm, Sweden
- USTUTT – Stuttgart, Germany



## CRESTA objectives and outputs

- Objectives
  - Progress state of the art research in exascale development
  - Develop and produce software for future exascale platforms
  - Enable a set of key *co-design* applications for exascale
  - Demonstrate the success of the co-design process
- Major outputs
  - The CRESTA research portfolio
  - The CRESTA systemware software collection
  - The CRESTA co-design applications
  - The CRESTA co-design methodology, tried and tested
- Concepts
  - Co-design
  - Disruptive vs incremental approaches

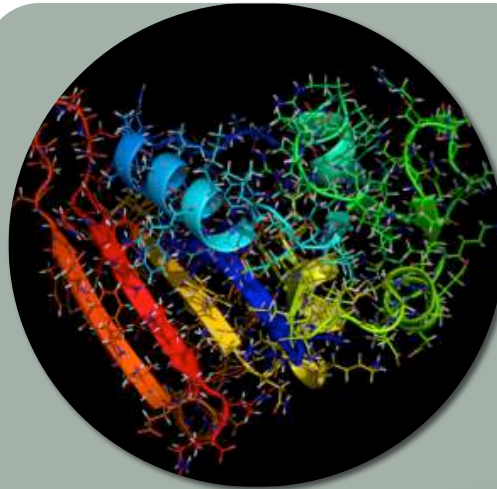
## Co-design applications



### Elmfire

Gyrokinetic code for turbulent fusion plasma  
 Simulating plasma behavior in large scale fusion reactors

An almost complete code restructuring  
 Radical reduction of memory consumption per core



### GROMACS

Molecular dynamics for

- Modelling of biological systems
- computational material and drug design

10M atom simulation

Coupling strong scaling techniques with ensemble scaling

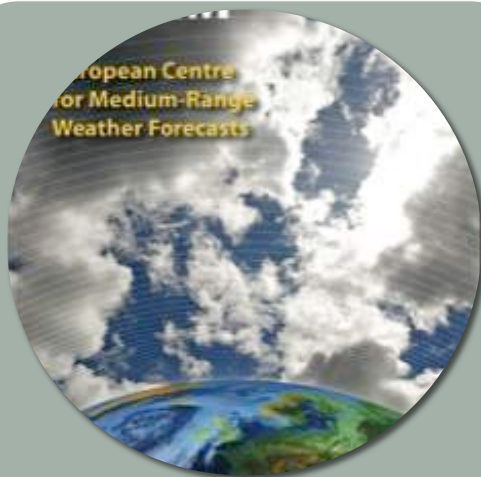


### HemeLB

Simulation of cerebrovascular bloodflow, using LB  
 Medical simulations to help surgeries  
 Brain aneurysm simulation

Pre- and post-processing and load balancing, LB dev  
 Hybridisation, restructuring

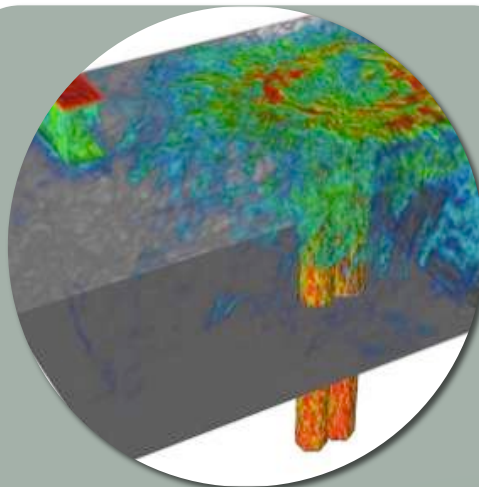
## Co-design applications



### IFS

Numerical weather prediction  
Timely and accurate weather forecasts can save lives  
Simulating the trajectory of hurricane Sandy

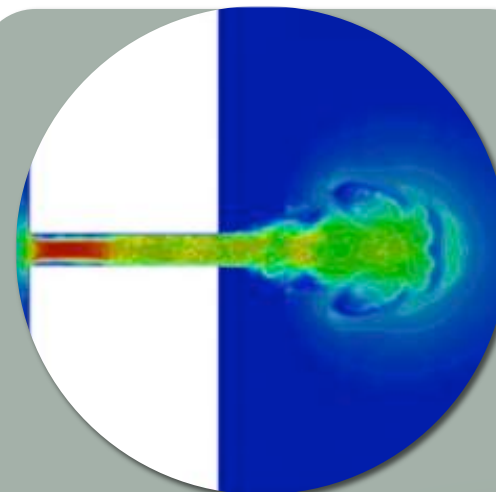
Acceleration  
Task-graph based parallelization  
New communication models



### Nek5000

Open-source CFD  
Scaled to 1M cores on Mira  
Nuclear power plant cooling simulations

Adaptive mesh refinement  
acceleration

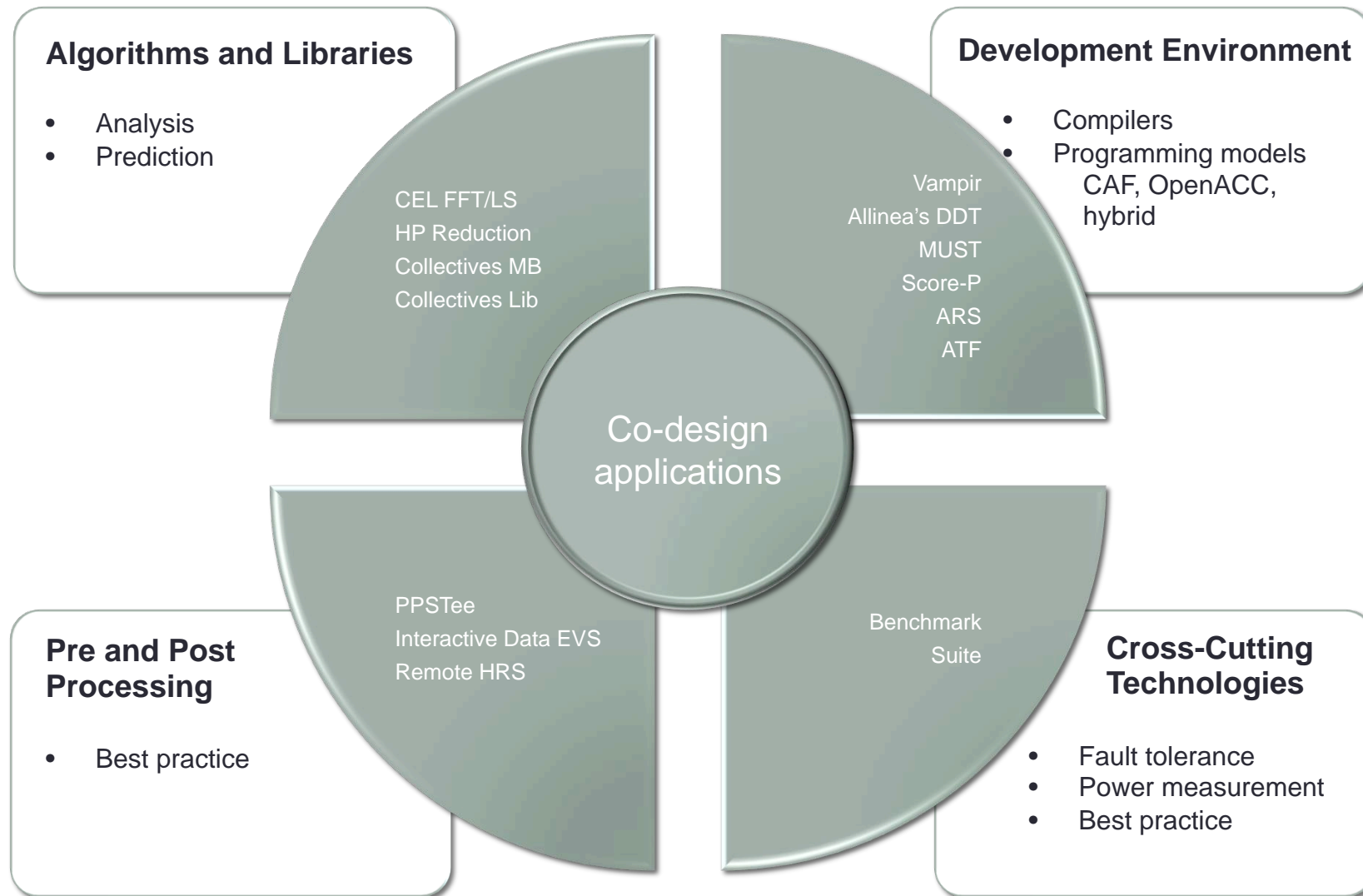


### OpenFOAM

Open-source CFD  
Turbulence models: fine resolution in space and time  
Wind turbines, hydroelectric power plants  
Francis pump turbine simulation

Linear solver optimization

# CRESTA software and research portfolio





# Concepts



## Co-design

Recognises the need to include all relevant perspectives and stakeholders in the design process

CRESTA is a showcase for the co-design methodology

CRESTA has a series of co-design teams cross-cutting WPs

Series of co-design specific success metrics

Needs to be benefit for *both* software developers and for application developers

Needs to show the whole is greater than the sum of its parts



## Disruptive vs incremental

Applications and systemware have made some major disruptive decisions within CRESTA

Disruptive technology meetings explore potentially disruptive solutions

## Key outputs and their success metrics

- Applications
  - Exploit largest systems possible today: performance/ functionality demonstrations
  - Regularly updated set of roadmaps –relevance for anticipated future exascale systems
  - Socio-economic advances –exemplar simulations with real scientific advances
- Systemware
  - Exploit largest systems possible today: performance/ functionality demonstrations
  - Enhanced roadmaps, driven by exascale requirements
  - Demonstrators with co-design applications
- Research portfolio
  - Published techniques and solutions to exascale challenges
  - Exploitation of techniques within co-design applications
  - Influence of community initiatives e.g. standard bodies
- Co-design
  - Systemware/research integrated into applications and application driven enhancements to systemware/research outputs
  - Both sets of roadmap enhanced through feedback from the other



## Impact and exploitation outputs and success metrics

- Series of high level impacts
  - Enhancing European leadership in HPC system software and tools, exascale simulation, and industry
  - Enhanced productivity of European scientists
  - Impact on socio-economic issues
- CRESTA's major impact outputs include
  - The EASC conference series
  - Special journal edition
  - Pilot study programme
  - Socio-economic impact videos
  - High impact journal publications
  - Workshop and training courses
  - Case studies and white papers
  - Significant targeting of SC and ISC
- Collaboration with other European exascale projects
  - E.g this meeting - we are very glad to see you all in Edinburgh
  - And collaboration more widely



## Conclusion

- CRESTA aims to:
  - Progress state of the art research in exascale development
  - Develop and produce software for future exascale platforms
  - Enable a set of key *co-design* applications for exascale
  - Demonstrate the success of the co-design process
- All co-design applications have made significant progress
  - Disruptive decisions a success in their own right
- Systemware software
  - All have prototype releases, working towards final releases
- Co-design
  - Series of examples of both the applications and the systemware benefitting
  - Case study series showcasing this success
- Impact
  - Creating impact across European industry, simulation software and with European scientists
  - Demonstrating leadership and engagement more widely: this is a *global* challenge