CCP5 Collaborative Computational Project Computer Simulation of Condensed Phases 40th Anniversary ++

AGENDA

16th of January

13:00 - 13:30 Lunch

13:30 - 14:30 Current status and news - Paola Carbone, Manchester, Chair of CCP5

14:30 - 15:30 Summer School + discussions - Colin Freeman, Sheffield, Chair of CCP5 Summer school

15:30 - 16:00 Coffee

16:00 - 16:30 MolSSI – Daniel Crawford, Virginia Tech, Director of MolSSI

16:30 - 18:00 Panel on creating community grants, Paola Carbone

19:00 - Dinner

17th of January

9:30 - 10:00 Excalibur - Scott Woodley, UCL, Chair of MCC

10:00 - 11:00 Software community needs discussion - Alin Elena, STFC, Secretary of CCP5

11:00 - 11:30 Coffee

11:30 – 12:00 PSDI/NDI - Barbara Montanari, STFC, Director of CoSeC

12:00 – 12:30 CECAM – Sara Bonella, Deputy Director of CECAM

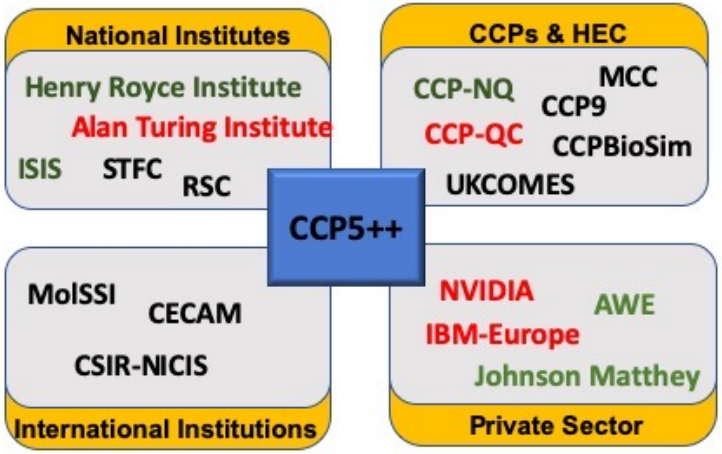
12:30 - Lunch

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Integrating Computer Simulation of Condensed Phases with Experiments and Data Science

Starting date 01/09/2021 three years project



Royce Institute*	**Alan Turing Institute***	**STFC***	**ISIS***	**RSC***
CCP-QC**	CCPNQ**	CCPBioSim**	CCP9**	
MCC**	UKCOMES**	CECAM*	CSIR-NICIS**	MolSSI**
IBM-Europe*	AWE**	NVIDIA**	Johnson Matthey*	

*Member of the Steering or Executive Committee and/or provide support to co-organize workshops and training activities (in addition to the project partners letters of support, see Letter of support from the Alan Turing Institute).
** Provide match-funding to run some of the network events.

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Network Structure

Chair: Paola Carbone, **Secretary and CoI**: Alin Elena

Steering committee:
Karen Edler , Gábor Csányi, Fernando Bresme, David Quigley, Richard Catlow, Peter Haynes, Jon Rowe, John Harding, Mark Wilson, Ignacio Pagonabarraga, Tristan Youngs, Barbara Montanari, James Elliott, Fausto Martelli, Misbah Sarwar

meet formally once a year. The steering committee will (*i*) review the structure of the network and training activity; (*ii*) monitor milestones and deliverables; (*iii*) approve changes in the executive committee members.

Executive committee:
Chris Lorentz,
Fernanda Duarte Gonzales,
Flor Siperstein,
Jonathan Skelton,
Andrew Logsdail,
David Wilkins
Mark Storr (Industrial rep)

run the network programme and administer its resources

Summer School committee:
Colin Freeman, Neil Allan, Alin Elena
+ Mark Miller

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Themes

Experimentally informed simulations (Theme Leads: Karen Edler)

Data-aided molecular simulations (Theme Lead: Gábor Csányi)

Novel algorithms in molecular simulations (Theme Lead: Fernando Bresme)

A UK landscape for materials simulation software (Theme Lead: David Quigley)

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The objectives of *CCP5++*

1) Identify the new grand-challenges in molecular modelling of materials;

2) Develop them into research programmes by sponsoring events and inter-disciplinary collaborations to nurture partnerships between experimentalists, simulators and data scientists;

3) Construct a roadmap for UK software development to link simulations and data analytics, working in partnership with the Alan Turing Institute and key national experimental facilities;

4) Sponsor knowledge transfer to the industrial sector including SMEs;

5) Develop long-lasting international collaborations with centres/institutes with similar remit (MolSSI, NICIS, CECAM);

6) Develop innovative approaches to training the next generation of molecular modellers.

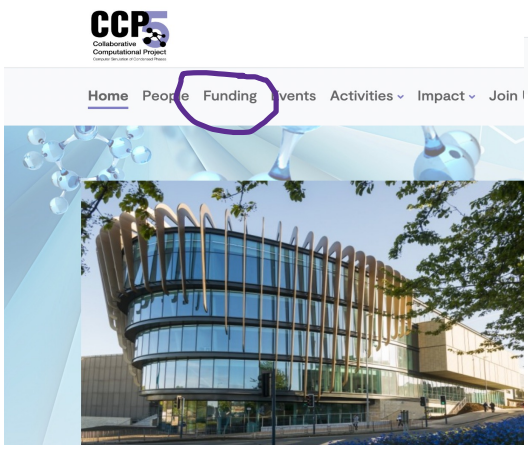
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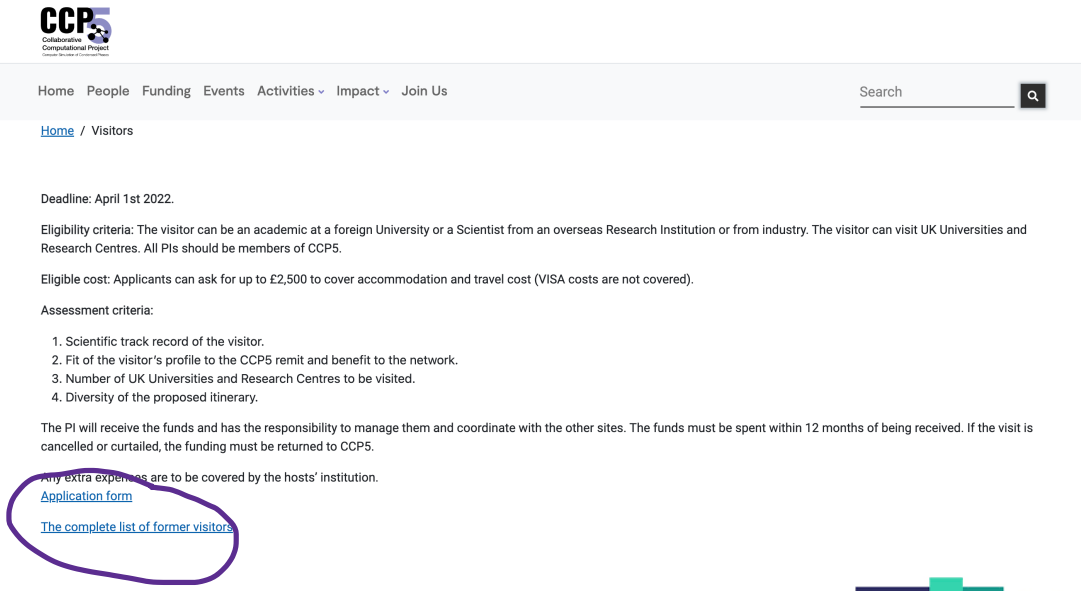
CONCLUSIONS FROM LAST YEAR MEETING

- Important to keep CCP5 identity. Perhaps expand to engineering community working on molecular modelling (adsorption, fluids). Mechanism to achieve it not clear other than supporting workshops.
- Idea to identify champions for specific areas however difficulty to ensure engagement
- Increase presence on social media to enhance visibility
- Increase engagement with RSC and other organization, common events
- Engage more closely with the tier2 HPC.
- Unclear what is now “community software”. Suggestion to run a proper survey
- Engagement with SME important but must be objectives-driven
- Importance of quality of website and brand
- Organize thematic workshops linked to the themes and led by the theme leads

DELIVERABLES

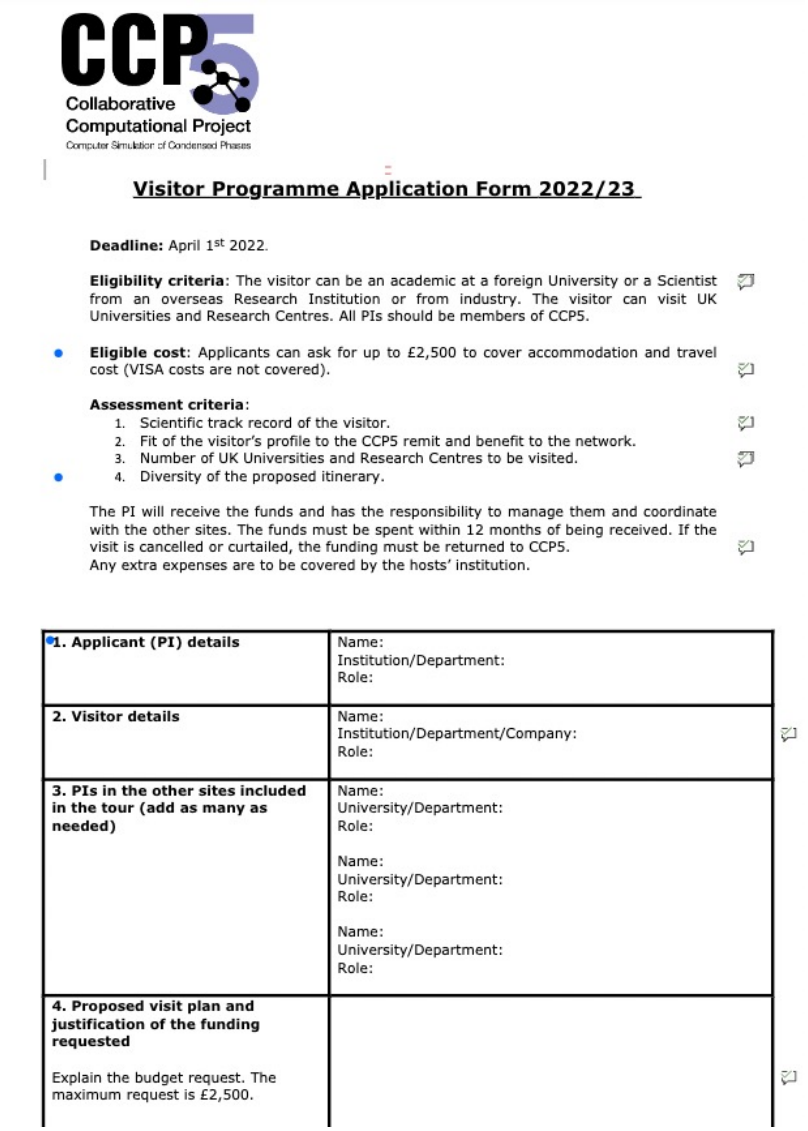
Deliverables for the coordination of the network	Target Objective	Due Date	
Set up of the steering committee	ALL	M2	✓
Set up website and brand	ALL	M2	✓
Establish calendar for call for network activities	ALL	M2	✓





± Activity revised every 6 months

DELIVERABLES



Collaborative Computational Project
Computer Simulation of Condensed Phases

Visitor Programme Application Form 2022/23

Deadline: April 1st 2022.

Eligibility criteria: The visitor can be an academic at a foreign University or a Scientist from an overseas Research Institution or from industry. The visitor can visit UK Universities and Research Centres. All PIs should be members of CCP5.

Eligible cost: Applicants can ask for up to £2,500 to cover accommodation and travel cost (VISA costs are not covered).

Assessment criteria:

1. Scientific track record of the visitor.
2. Fit of the visitor's profile to the CCP5 remit and benefit to the network.
3. Number of UK Universities and Research Centres to be visited.
4. Diversity of the proposed itinerary.

The PI will receive the funds and has the responsibility to manage them and coordinate with the other sites. The funds must be spent within 12 months of being received. If the visit is cancelled or curtailed, the funding must be returned to CCP5.
Any extra expenses are to be covered by the hosts' institution.

1. Applicant (PI) details	Name: Institution/Department: Role:
2. Visitor details	Name: Institution/Department/Company: Role:
3. PIs in the other sites included in the tour (add as many as needed)	Name: University/Department: Role: Name: University/Department: Role: Name: University/Department: Role:
4. Proposed visit plan and justification of the funding requested Explain the budget request. The maximum request is £2,500.	

± Activity revised every 6 months

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DELIVERABLES

Cross community **CCP5 community** **Industrial engagement**

Deliverables for the network	Due Date	
Identify 3 grand challenges in materials modelling	M12±	
Organize 2 training activities with ISIS	M12 revised M24	
Support 4 workshop/sandpits in collaboration with ATI and Royce Institute	M12 revised M24	✓
Organize 1 community led workshops/sandpits on algorithms and modelling techniques per year	M12+	✓
Support 5 UG internships per year	M12+	✓
Coordinate 1 industry day and 2 postgrad secondments per year	M20 revised M36	✓
Support 1 international visitor per year	M12+	
Organize tutorials for industry and experimental community	M12+	
Organize 1 coding workshop per year	M12+	
Coordinate network activities together with existing CCPs and consortia	M12+	✓
Organization of the annual summer school	M12, M24, M36	✓
Storage of all training materials and publication online	M12+	

± Activity revised every 6 months

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DELIVERABLES

CCP5 community

- Run the first face-to-face summer school in two years in Durham. Highly subscribed (204 applications for 70 places!)



- Award two CCP5 prizes in 2019 (Kostya Trachenko, QMUL) and the 2022 (Colin Freeman, Sheffield)
- Award the first CCP5/CECAM sandpit project (Nicodemo Di Pasquale, Brunel)
- Award the first PhD placement bursary (Amit Chaudhari, Cardiff-JM)
- Award 5 UG summer bursaries (all to new applicants)
- Run 1st face-to-face AGM in Huddersfield 2022.

DELIVERABLES

Cross community activities

- Run the biennial CCP5-CCPBioSim Multiscale simulation in Manchester (April 2023)
- Co-sponsor with CCP-NC a cross community meeting in 2023 on Disordered materials (Paul Hodgkinson/Fred Blanc / Vasily Oganesyan + David Quigley CCP5)
- Co-sponsor with Royce ”ML in materials” March 2023 (Alin Elena/Kim Jelfs/Keith Butler)
- Co-sponsored the MMMHub ++ online conference in 2021
- Discussion on co-organizing a large Molecular Simulations conference with all CCPs and HECs involved 2023 or 2024

DELIVERABLES

Industrial engagement

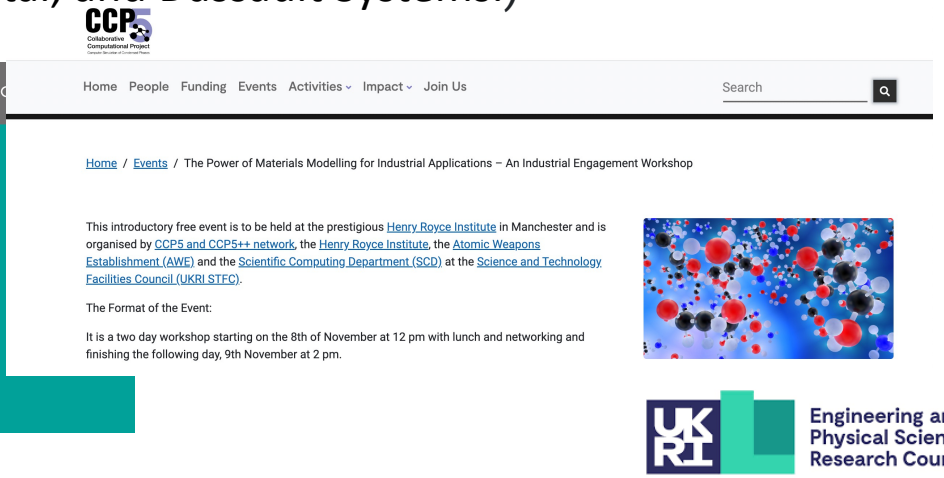
Co-sponsored with Royce Institute, AWE and STFC (November 2022)

The aim of this workshop is to:

- share knowledge and awareness of the materials modelling endeavours supported by CCP5 that are of benefit to UK PLC,
- hear from our industrial partners impact this has brought to their industry
- round table discussion

(attendees from: GSK, DSTL, National Nuclear Lab, Victrex, Synbiosis Ltd, Concrete4Change Ltd, AWE, Johnson Matthey, IBM, Continental, and Dassault Systems.)





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DELIVERABLES

Cross international community activities

With CECAM

- Set up a memorandum of understanding with CECAM
- Open the first call for the CCP5/CECAM sandpit



DELIVERABLES

Cross international community activities

With CSIR-NICIS (HPC center South Africa)

- Invitation of director Dr Happy Sithole to the AGM in Huddersfield (September 2022)
- Invited talk to CHPC NICIS national conference in Pretoria (November 2022)
- Initial meeting on the usage of DL_POLY, interested in supporting for software and in training activities



DELIVERABLES

Grants writing and involvement

Submitted “Software for community” grants directly benefitting CCP5:

- **Developing next-generation DL_POLY for the benefit of the modelling community (QMUL, STFC) (successful)**
- Integration of machine learning interatomic potentials into molecular dynamics software **(UoM, STFC, Cambridge) (unsuccessful)**

Wrote 7 letters of support.

Other grants related to CCP5:
CASTEP-USER: Predictive Materials Modelling For Experimental Scientists (York)
Supporting research communities with large-scale DFT in the next decade and beyond (Southampton)
CP2K For Emerging Architectures And Machine Learning (Lincoln)
Supporting the OpenMM Community-led Development of Next-Generation Condensed Matter Modelling Software(Edinburg)

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++ CRITICAL SUCCESS FACTORS

Critical success factors	Due Date
Widening participation: increase membership from SMEs, experimentalist and data scientists	M20 revised M36
Secure financial support from existing and new partners towards partial self-sustainability	M24 revised M36
2 grant proposals submitted	M24 revised M36
New UK software roadmap supported by EPSRC	M24 revised M36
3 AGM with high attendance from wider community	M12, M24, M36
Support to individuals for fellowship applications in the area of materials modelling	M12, M24, M36

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FINANCE

Event	Cost/k £	Details	Comments
Summer school	60		1 per year
Coding days	12		2 per year
Industry days	6		1 per year
Workshops	12		around 3 per year
Sandpits	24		1 per year with CECAM
Planned events	14		CCPBioSim 3.5k + 7 pre-agre
AGM	24		1 per year
CCP5 Prize	6		every two years
Postgrad support	24		4k pa 2 each year
UG bursaries	45		5 per year
TOTAL directly Incurred	**227**		
Visitor Programme	7.5		1 per year
TOTAL	**234.5**		

Travel Costs	
Committee meetings	18.00
Travel costs	5.00
TOTAL Directly Incurred	**257.50**

A	**EPSRC - UoM**	**310,155.81**	**53,337.68**	**-**	**256,818.13**	**17%**
A05	Travel and subsisten	34,045.65	698.08	-	33,347.57	2%
A07	Consumables	268,808.10	49,799.98	-	219,008.12	19%

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Point of discussion

Collaborations:

- ❑ *Strengthen link with Royce (could this year conference become a feature?)*
- ❑ *Initiate collaboration with ATI*
- ❑ *Maintain collaboration with CECAM*
- ❑ *Establish collaboration with the computational centre in South Africa for software support.*
- ❑ *Explore possibilities with MOLSSI*

Visibility/engagement:

- ❑ *Ensure people that get funded acknowledge us*
- ❑ *Strengthen our presence on twitter*
- ❑ *Report on funding received published on the website*
- ❑ *Organize CCPs/HECs molecular modelling conference*
- ❑ *New type of workshop/training? Target workshop for students?*

Points of discussion

Software: Focus group on software strategy. Do we need one?
More link with the Tier 2 HECs? More engagement with ARCHER consortia?
How is our usage of ARCHER2?

Engagement with existing activities:

- ❑ *PSDI*
- ❑ *Excalibur*

Future fundings

- ❑ *AI Hubs*
- ❑ *CDTs*

- ❑ *How to manage letters of support?*

Summary of the meeting and actions

PC: Paola Carbone, AME: Alin Elena, FC: Colin Freeman, NA: Neil Allan.

Collaboration with SA: There is an interest to run a tailored summer school with NSIC. JM has several sites there, they are interested to be involved. We can use CCP5++ money to support exchange of students/PIs to establish collaborations on key areas.
Action PC, AME: contact Happy Sithole to discuss how to proceed.

Summer School: doing well, need to find host for next year. Chris Lorentz will investigate, possible use of a site in the Lake district managed by U. Cumbria, last resort Telford. Contact in Lincoln. Need to find industrialist for the summer school. Someone was suggested but I do not have the name. Fausto and Gabor and Chris suggested names. Suggestion to use the contact list collected for the Royce meeting.
Action AME, FC, NA: contact possible hosts for next year, contact Fausto, Gabor and Chris for suggestion of names.

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Summary of the meeting and actions

Replacement of Karen Adler as theme lead for experiment theme. Various names suggested: Andy Parnell (Sheffield), Alison ? Cardiff, Loren Dugan (Leeds). Karen and Tristan will suggest more names.
Action AME, PC: collect names and preference, and contact the person (by March)

Collaboration with ATI: successful bid for a workshop should include biophysics as they are already working on it data driven simulations. Contact Sarah. Possibly better to wait for deadlines of AIHub and CDT.
Action PC, AME: postponed.

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Summary of the meeting and actions

Collaboration with MOLSSI: seems most of the effort has been spent so far in the electronic structure calculations. Possible avenues is to collaborate on standardization or workflow design for highthroughput classical simulation. Need to set up an intial online meeting (ask who wants to be involved).
Action (PC, AME): contact Daniel Crawford to set up an online meeting. Identify CCP5 people that could be involved in the discussion (theme leads). Relation with the possible grant.

CECAM collaboration: for the summer school and research: current projects recent funded EU grant MultiXscale, Lhumos with Max for pre-developed training materials (CCP5 summer school?), Oscar for support materials for teaching modelling via notebooks (CCP5 summer school?)
Action (PC): discussion with Sara Bonella to possible involvement in other CECAM project. Discuss with Colin and Alin about possible use of teaching platform for summer school.

Summary of the meeting and actions

Royce: AIHubs macrostructure, ML potentials. **No action**

International conference on modelling: with all CCPs and HECs on molecular modelling and STFC. The committee members were positive. Most suited date would be 2024 due to international conference on materials in Dublin in 2023. Barbara expressed support for such initiative.
Action PC, AME: to contact again chairs CCPs, HECs to organize an online meeting.

Action AME: Ask speakers if they can share the slides. Create link on website to submit files and create accounts.

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Summary of the meeting and actions

Possible grant (need discussion with EPSRC about what is the best call for this grant. Elisabeth Bent):

1) Interoperability with various MD software to exploit the strengths of each (interoperability between codes and methods)
2) Benchmarking for proper interoperability is a must
3) Work with MolSSI for I/O (NOMAD, ASE, Aiida, ST4ST)?
4) Analysis tools

5) Exascale link: if we go for GPUs what is still unsolved is multinode GPUs (this is code agnostic)
6) Postprocessing analysis is key for classical simulation in addition to choice of force field. The first is difficult to automate but postprocessing can be. Existing effort from IBM to develop post-processing platform ST4SD which is open-source. We could link with them.
7) Ada Lovelance centre a possible way for funding?