



**E-Infrastructures
H2020-EINFRA-2015-1**

**EINFRA-5-2015: Centres of Excellence
for computing applications**

**EoCoE
Energy oriented Center of Excellence
for computing applications**

Grant Agreement Number: EINFRA-676629

**D6.5 - M36
Third annual thematic workshops report - Year 3**

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* - The dissemination level are indicated as follows: PU – Public, CO – Confidential, only for members of the consortium (including the Commission Services) CL – Classified, as referred to in Commission Decision 2991/844/EC.

Document Control Sheet

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1. Background

Task 6.1.6 of the EoCoE project consists in organising a series of 9 thematic workshops to present research products to the other project partners. Project partners are expected to propose workshop themes based on outputs from the different work packages. These workshops can also be open to the wider end-user community. In Year 3, 8 workshops were organized, which are described below.

WP	Workshop	Dates	Place	Registrants	Indus. regist.	Attendees
WP1	Scientific Applications toward Exascale	4-5 Oct. 2017	CINES (Montpellier, France)	45		45
WP5	NumKin	23-27 Oct. 2017	IPP (Garching, Germany)	57		57
WP6	HPC4RE (SC17)	14 Nov. 2017	Colorado Convention Center (Denver, USA)			15
WP5	Eurofusion	27-29 Nov. 2017	Sheraton Dubrovnik Riviera Business Hotel (Dubrovnik, Croatia)			
WP1	Training in Parallel I/O" w systemach i aplikacjach HPC	11-14 Dec. 2017	PSNC (Poznan, Poland)	17		17
WP3	EoCoE Workshop in EERA Joint Program	15 Dec. 2017	Hotel Royal Continental (Naples, Italy)	23	3-4	23
WP6	EoCoE-Ampea Workshop	7 June 2018	EERA (Brussels, Belgium)	26	1	24
WP1	Hackathon	11-13 June 2018	Maison de la Simulation, CEA (Paris-Saclay, France)	16		15
WP3	EMRS Conference	18-22 June 2018	Strasbourg Convention Center (Strasbourg, France)		6	146
WP1	First EoCoE Webinar	31 May 2018	GoToWebinar	21		17
WP1	Second EoCoE Webinar	14 June 2018	GoToWebinar	36		26
WP3	Third EoCoE Webinar	11 June 2018	GoToWebinar	11		6
WP4	Fourth EoCoE Webinar	11 September 2018	GoToWebinar	70		43
WP5	Fifth EoCoE Webinar	25 September 2018	GoToWebinar			

Table 1: EoCoE Third Year Workshops

2. Scientific Applications toward Exascale

2.1 Aims

During the first day-and-half of this workshop, 17 talks have been presented in total. The 45 participants could get an update on the current and coming European HPC landscape. They could also hear the lessons learned by researchers that have ported and tested KNL and GPU architectures.

The last day was dedicated to a hands-on session on the PRACE PCP machine hosted at CINES based on the Intel Xeon Phi KNL architectures. The 18 participants could port their codes and produce their first energy measurement.

The global feedbacks from the participants are very positive, we can consider the workshop as a success !

2.2 Agenda

Wednesday October 4th 2017

- 09:00 Welcome + coffee
- 09:20 EoCoE project, Edouard Audit (MdlS)
- 09:30 PRACE PCP CINES, Olivier Rouchon (CINES)
- 09:50 KNL architecture, Asma Farjallah (Intel)
- 10:20 Towards energy consumption application profiling with BULL energy software France Boillod-Cerneux (Atos)
- 10:50 Break
- 11:20 GENCI technological survey group, Gabriel Hauteux (GENCI)
- 11:40 CINECA Marconi, Carlo Cavazzoni (CINECA)
- 12:00 Optimizing Electronic-Structure Codes for KNL: Lights and Shadows, Pietro Bonfa' (CINECA)
- 12:30 Lunch break
- 14:00 Towards Green Aviation with Python at Petascale, Peter Vincent (Imperial College London) Gordon Bell finalist 2016
- 15:00 qr_mumps: a runtime-based Sequential Task Flow parallel solver, Alfredo Buttari (IRIT)
- 15:30 Efficient Monte Carlo Neutron Transport Calculations with Advanced Architectures, Yunsong Wang (MdlS)
- 16:00 Break
- 16:30 Metalwalls on Xeon, Xeon Phi and GPU, Matthieu Haefele (MdlS)
- 17:00 Porting of Alya, a high performance computational mechanics code, to accelerators: KNL and GPU, Herbert Owen (BSC)
- 18:00 Bus to the social event

Thursday October 5th 2017

- 09:00 DEEP-EST Project - A different take on Heterogeneous Cluster Architectures Norbert Eicker (JSC)

09:30 Fusion energy and the case for exa-scale computing , Steve Lisgo (ITER)
10:00 Scaling and optimizing Gysela code on a Intel KNL cluster, Guillaume Latu (CEA)
10:30 Break
11:00 PIC codes on the road to exascale: adaptation to MIC architectures, Mathieu Lobet (MdlS)
11:30 POP performance auditing of applications on new architectures, Brian Wylie (JSC)
12:00 Lunch break
13:30 Lectures on PRACE PCP and KNL usage
14:30 KNL Hands-on (4h)

Friday October 6th 2017

09:00 KNL Hands-on
12:00 Lunch break

2.3 Pictures



Figure 1: Scientific Application towards Exascale Workshop

2.4 List of participants

See the list of participants here next page.

non-eocoe

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2.5 Core metrics of the Workshop

Date: 4-5 October 2017

Location: CINES, Montpellier (France)

Number of registrants: 45

Industrial registrants: 0

Number of attendees: 45

3. Numkin Workshop

3.1 Aims

The purpose of this workshop is to bring together a small number of specialists in the development of numerical methods for collisionless and collisional kinetic equations, and discuss the current evolutions in the field. It was also the annual general meeting of the EUROfusion Enabling Research project on Verification and development of new algorithms for gyrokinetic codes and a meeting of the EUROfusion Enabling Research project on Turbulent and Neoclassical Transport in tokamak plasmas (TNT). There was also a meeting of the Work package on Fusion of the Energy Oriented Center of Excellence (EoCoE) established within the Horizon 2020 programme of the European Commission.

3.2 Agenda

Monday, October 23rd

08:00 Registration at IPP, Building D2, ground floor

08:45 Welcoming

09:00 Helluy, Philippe - Palindromic Discontinuous Galerkin Method

09:35 Discussion

09:45 Filbet, Francis - Particle methods for the three dimensional Vlasov-Poisson system with a large magnetic field

10:20 Discussion

10:30 Coffee break

11:00 Kraus, Michael - Metriplectic Integrators for the Landau Collision Operator

11:35 Discussion

11:45 Ameres, Jakob - Stochastic and Spectral Particle Methods for Plasma Physics

12:20 Discussion

12:30 Lunch break

14:00 Kormann, Katharina - Semi-implicit time stepping for finite element particle-in-cell methods

14:35 Discussion

14:45 Campos-Pinto, Martin - Adding smooth resamplings to particle codes

15:20 Discussion

15:30 Coffee break

16:00 Negulescu, Claudia - Kinetic modelling and numerics of strongly magnetized tokamak plasmas with mass disparate particles. The electron Boltzmann relation.

16:35 Discussion

16:45 Bostan, Mihai - On the asymptotic analysis of parabolic equations with stiff transport terms

17:20 Discussion

Tuesday, October 24th

09:00 Hesthaven, Jan - Hierarchical Model Development for Uncertainty Quantification in Complex Systems

09:35 Discussion

09:45 Despres, Bruno - Uncertainty propagation

10:20 Discussion

10:30 Coffee break

11:00 Poette, Gael - Uncertainty quantification for complex flows: a brief state of the art on spectral methods and examples

11:35 Discussion

11:45 von Toussaint, Udo - Uncertainty Quantification: Polynomial Chaos Expansion based approaches: Prospects and Limitations

12:20 Discussion

12:30 Lunch break

14:00 Leerink, Susan

Full f gyrokinetic ELMFIRE simulation including kinetic electrons

14:35 Discussion

14:45 Tronko, Natalia - Theory and numerical simulations for verification of gyrokinetic codes

15:20 Discussion

15:30 Coffee break

16:00 Biancalani, Alessandro - Results of the verification and benchmark of GK codes on GAMs obtained in 2017

16:35 Discussion

16:45 Bottino, Alberto - Toward global full-f electromagnetic gyrokinetic PIC simulations

17:20 Discussion

Wednesday, October 25th

09:00 Garbet, Xavier - Enabling Research TNT session opening

09:15 Tronko, Natalia - Introduction

09:40 Discussion

09:50 Donnel, Peter - A multi-species collision operator for gyrokinetic codes: Validation with the code GYSELA

10:15 Discussion
 10:25 Coffee break (20 min.)
 10:45 Mauriya, Adwiteey - Upgrading the GS2 collision operator
 11:10 Discussion
 11:20 Scheinberg, Aaron - Benchmarking and recent development for ORB5's single- and multi-species collision operators
 11:45 Discussion
 11:55 Crandall, Paul - Extension of the GENE collision operator model
 12:20 Discussion
 12:30 Lunch break
 Afternoon free
 19:00 Social dinner at the "Garchinger Augustiner" - Freisinger Landstr. 4, 85748 Garching

Thursday, October 26th

Enabling Research Project TNT (parallel session)
 (D2 Lecture hall)

09:00 Caschera, Elisabetta - Scaling of confinement time and SOL-like boundary conditions in GYSELA global and flux-driven simulations
 09:35 Discussion
 09:45 Peeters, Arthur - Magnitude of the neo-classical driven momentum flux
 10:20 Discussion
 10:30 Coffee break
 11:00 Idouakass, Malik / Gravier, Etienne - Impurity transport modeled with the TERESA code
 11:35 Discussion
 11:45 Garbet, Xavier - Impact of poloidal asymmetries on transport
 12:20 Discussion
 12:30 Lunch break

EoCoE(parallel session)
 (D2 Seminar room, 2nd floor)

09:00 Sarazin, Yanick - Introduction
 09:10 Ratnani, Ahmed - Towards an automated mesh generation framework for Tokamaks
 09:40 Discussion
 09:45 Hendrik, Speleers - A framework for isogeometric analysis on unstructured quadrilateral meshes
 10:15 Discussion
 10:20 Coffee break (25 min.)
 10:45 Lakhlili, Jalal - Mesh generation with isogeometric approach for 2D tokamak equilibria
 11:15 Discussion

11:20 Latu, Guillaume - Scaling and optimizing Gysela code on an Intel KNL cluster

11:50 Discussion

11:55 Marandet, Yannick - Effect of statistical noise on coupled plasma fluid – Monte Carlo kinetic neutrals

12:25 Discussion

12:30 Lunch break

Afternoon session
(D2 Lecture hall)

14:00 Ghendrih, Philippe - PoPe verification and model reduction scheme: application to 1D-1V multispecies kinetics

14:35 Discussion

14:45 Crestetto, Anaïs - A particle-based micro-macro decomposition for Boltzmann-BGK-like equations in the diffusion scaling

15:20 Discussion

15:30 Coffee break

16:00 Güçlü, Yaman - Semi-Lagrangian drift-kinetic simulations in toroidal geometry

16:35 Discussion

Friday, October 27th

Selalib Day - Seminar room on 2nd floor

10:30 Coffee break

12:00 Lunch break

3.3 Pictures

N/A

3.4 List of participants

See the list of participants next page.

3.5 Core metrics of the Workshop

Date: 23-27 October 2017

Location: IPP (Garching, Germany)

Number of registrants: 57

Industrial registrants: unknown

Number of attendees: 57

Arrived:

"yes" to Social Dinner 25.10.

	Ameres	Jakob	S	23/10/2017	27/10/2017			
	Biancalani	Alessandro	S	23/10/2017	27/10/2017	TOK		
	Bostan	Mihai	S	23/10/2017	26/10/2017	Hoyacker Hof	Aix-Marseille U.	
	Bottino	Alberto	S	23/10/2017	27/10/2017	TOK		
	Bressan	Camilla		23/10/2017	27/10/2017			
	Brunner	Stephan		24/10/2017	26/10/2017	Hoyacker Hof	EPFL Lausanne	
	Campos Pinto	Martin	S	22/10/2017	27/10/2017	Hoyacker Hof	UPMC Paris	
	Caschera	Elisabetta	S	22/10/2017	27/10/2017	Hoyacker Hof	CEA, Cadarache	
	Crandall	Paul	S	25/10/2017				
	Crestetto	Anaïs	S	22/10/2017	27/10/2017	Hoyacker Hof	UFR Nantes, FR	
	de Oliveira	Felipe Nathan		zeitweise		TOK/PhD student		
	Despres	Bruno	S	22/10/2017	27/10/2017	Hoyacker Hof	UPMC Paris	
	Dodhy	Adila		23/10/2017	27/10/2017			
	Donnel	Peter	S	23/10/2017	27/10/2017	Hoyacker Hof	CEA, Cadarache	
	Fedele	Baptiste		22/10/2017	27/10/2017	Hoyacker Hof		
	Filbet	Francis	S	22/10/2017	26/10/2017	Hoyacker Hof	Univ. Toulouse	
	Franck	Emmanuel		23/10/2017	27/10/2017	n/a		
	Frank	Alexander		23/10/2017	27/10/2017	Masterstudent-IPP		
	Garbet	Xavier	SO	23/10/2017	26/10/2017	Hoyacker Hof	CEA, Cadarache	
	Ghendrih	Philippe	S	22/10/2017	27/10/2017	Hoyacker Hof	CEA, Cadarache	
	Grandgirard	Virginie		23/10/2017	27/10/2017	Hoyacker Hof		
	Gravier	Etienne	S	25/10/2017	26/10/2017	n/a	Univ. Lorraine	
	Güclü	Yaman	S	23/10/2017	27/10/2017			
	Gutnic	Michaël		22/10/2017	27/10/2017	Hoyacker Hof		
	Hatzky	Roman		23/10/2017	27/10/2017			
	Hayward	Thomas		zeitweise		TOK		
	Helluy	Philippe	S	22/10/2017	27/10/2017	Hoyacker Hof	UNISTRA	
	Hesthaven	Jan	S	22/10/2017	24/10/2017	Hoyacker Hof	EPFL Lausanne	
	Hirstoaga	Sever		22/10/2017	27/10/2017	Hoyacker Hof		
	Hoelzl	Matthias		zeitweise		TOK		
	Idouakass	Malik	S	24/10/2017	27/10/2017	Hoyacker Hof	Univ. Lorraine	
	Kang	Kab Seok		23/10/2017	27/10/2017			

Arrived:

"yes" to Social Dinner 25.10.

	Kormann	Katharina	S	23/10/2017	27/10/2017		
	Kraus	Michael	S	23/10/2017	27/10/2017		
	Lakhlili	Jalal	S	23/10/2017	27/10/2017		
	Latu	Guillaume		23/10/2017	27/10/2017	Hoyacker Hof	
	Leerink	Susan	S	23/10/2017	26/10/2017	Aalto University	
	Maj	Omar		23/10/2017	27/10/2017		
	Marandet	Yannick	S	24/10/2017	26/10/2017	Hoyacker Hof	Aix-Marseille U.
	Mauriya	Adwiteey	S	22/10/2017	27/10/2017	Hoyacker Hof	IST, Lissaboon
	Murugappan	Moahan		zeitweise		Masterstudent-IPP	
	Navaro	Pierre		22/10/2017	27/10/2017		
	Negulescu	Claudia	S	21/10/2017	27/10/2017	Hoyacker Hof	Univ. Toulouse
	Nicolopoulos	Anouk (Ms)		23/10/2017	27/10/2017		UPMC Paris
	Peeters	Arthur	S	26/10/2017	26/10/2017	n/a	Univ. Bayreuth
	Poette	Gael	S	22/10/2017	26/10/2017	Hoyacker Hof	CEA, Arpajon
	Possanner	Stefan		23/10/2017	27/10/2017		
	Ratnani	Ahmed	S	23/10/2017	27/10/2017		
	Sarazin	Yanick	SO	23/10/2017	26/10/2017	Hoyacker Hof	CEA, Cadarache
	Scheinberg	Aaron	S	22/10/2017	27/10/2017	Hoyacker Hof	EPFL Lausanne
	Sonnendrücker	Eric	SO				
	Speleers	Hendrik	S	24/10/2017	27/10/2017	Hoyacker Hof	Univ. Rom
	Tronko	Natalia	S	23/10/2017	27/10/2017		
	von Toussaint	Udo	S	23/10/2017	27/10/2017		
	Xiong	Tao		23/10/2017	27/10/2017	n/a	Univ. Toulouse
	Yurova	Anna		23/10/2017	27/10/2017		
	Zoni	Edoardo		23/10/2017	27/10/2017		

4. HPC4RE

4.1 Aims

EoCoE held a networking meeting on the theme 'HPC for Renewable Energy' at the SC17 in Denver on Tuesday 14th of November, 1:30pm-3pm - Room 711.

By its nature renewable or low-carbon energy includes a wide spectrum of applications (wind, solar, battery storage materials, wave/tidal, nuclear fusion, etc) and algorithms with varying degrees of HPC maturity. The idea was to exchange experiences on this relatively new topic, to see if HPC can be leveraged to accelerate the global energy transition to RE, and conversely to find out to what extent RE is being used as a new driver for HPC in various countries around the world.

This event was organised by Edouard Audit and Paul Gibbon from the EoCoE project, Mitsuhsa Sato of the RIKEN Advanced Institute for Computational Science.

There followed a round-table discussion on possible follow-up actions, such as a BoF/workshop on HPC4RE at, for example the ISC'18 in Frankfurt. Slides of the talks will be made available shortly.

4.2 Agenda

- Edouard Audit, Maison de la Simulation: Summary of the EoCoE Consortium
- Happy Sithole, CHPC Cape Town, SA: Energy-HPC programs at CHPC
- Mitsuhsa Sato, RIKEN, Japan: FLAGSHIP 2020 project and Researches for energy problems using the Post-K supercomputer
- Alvaro Coutinho, HPCC, Rio de Janeiro: High Performance Computing for Energy (HPC4E Project)
- Andrea Quintiliani, ENEA, Rome: An overview of ENEA activities on Renewable Energies
- David Emerson, Daresbury: Delivering Energy-Related R&D Using Open-Source Software and High Performance Computing

4.3 Pictures

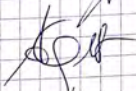
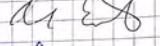
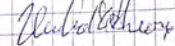
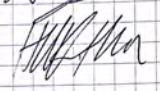
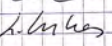
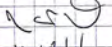
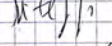
Here below a couple of pictures of the HPC4RE workshop.



Figure 2: Pictures of HPC4RE workshop

4.4 List of participants

HPC 4 R E - SC 17 - 14/11/2017
List of participants.

NAME	SURNAME	INSTITUTE	SIGN
SILVIO	MIGLIORI	ENEA	
ANDREA	QUINTILANI	ENEA	
ALBINO	AVELEDO	UFPR	
RICARDO	WAGAO	AMT	
MITSUKISA	SATO	RIKEN	
Adrian	Jackson	EPCC	
Michael	Hercux	US DOE, Sandia	
David	Emerson	STFC	
Happy	Sethole	CHPC	
Paul	Gibson	FZJ	
Linda	Geseke	UFPR	
ALVARO	COUTINHO	UFPR	
MARTA	MATTOSO	UFPR	
ANTONIO TADEU	GOMES	LNCC	
Nathalie	Girard	CEA	

Scanned with CamScanner

4.5 Core metrics of the Workshop

Date: 14 November 2017

Location: Supercomputing 17, Colorado Convention Center (Denver, US)

Number of registrants: 15

Industrial registrants: 0

Number of attendees: 15

5. EuroFusion

5.1 Aims

25th European Fusion Programme Workshop on "Numerical Modelling for Fusion", Dubrovnik, Croatia, 27-29 November 2017.

This EFPW was organised by Ruđer Bošković Institute (RBI) and Faculty of Electric Engineering, Mechanical Engineering and Naval Architecture of University of Split (FESB) on behalf of EUROfusion

The programme includes oral contributions from project members covering multi-scale modelling of plasma turbulence codes and Exascale computing. EoCoE partners will also participate in a round-table discussion on exascale computing for plasma physics applications. The meeting presents a good opportunity to disseminate work within EoCoE on plasma codes to the EUROfusion community.

5.2 Agenda

See the agenda here next page.

5.3 Pictures



Figure 3: Pictures of EFPW workshop

5.4 List of participants

N/A

5.5 Core metrics of the Workshop

Date: 27-29 November 2017

Location: Sheraton Dubrovnik Riviera Business Hotel (Dubrovnik, Croatia)

Number of registrants: unknown

Industrial registrants: unknown

Number of attendees: unknown

25th European Fusion Programme Workshop Draft Programme

Dubrovnik, Croatia

Numerical modelling for fusion

Monday 27 November 2017		
08:15	Welcome	
Session 1: Towards exascale computing		
08:30	Introduction	Eric Sonnendrücker (IPP)
08:40	Overview of hardware and software evolution towards exascale	Paul Gibbon (Jülich Supercomputing center)
09:10	Exascale challenges from site infrastructure and management perspective	Marcin Plociennik (PSNC)
09:40	Turbulence, core edge coupling	Frank Jenko (IPP)
10:10	Coffee Break	
10:30	Exascale computing for materials	Llion Evans (UKAEA)
11:00	Computer science aspects for exascale turbulence simulations	Guillaume Latu (CEA)
11:30	Discussion	
12:30	Lunch Break	
Session 2: Code validation		
14:00	Introduction	Roland Sabot (CEA)
14:15	Towards improved plasma confinement: Understanding plasma turbulence and self-organization via gyrokinetic modelling	Susan Leerink (VTT)
14:45	Validating models for energetic particle driven modes in the view of ITER and DEMO	Philipp Lauber (IPP)
15:15	Predict first: a pathway to fast full device modelling by combining validated reduced models and machine learning	Jonathan Citrin (DIFFER)
15:45	Coffee Break	
16:15	Dynamics of ELMs and their control methods: comparisons between experiments and modeling	François Orain (IPP)
16:45	Bridging SOL & edge theory and simulations to experiments: a mandatory confrontation	Philippe Ghendrih (CEA)
17:15	Discussion	
18:15	End	

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Tuesday 28 November 2017		
Session 3: Multi-scale physics for ITER		
08:15	Introduction	Paolo Ricci (SPC)
08:30	Approaching multi-scale and multi-physics issues for exhaust modelling	Jens Juul Rasmussen (DTU)
09:00	Approaching multi-scale and multi-physics issues for pedestal modelling	Howard Wilson (University of York / UKAEA)
09:30	Approaching multi-scale and multi-physics issues for core modelling	Yanick Sarazin (CEA)
10:00	Coffee Break	
10:30	Approaching multi-scale and multi-physics issues for runaways modelling	Tunde Fulop (Chalmers)
11:00	The challenge of integrating multi-scale and multi-physics in transport simulations	Gloria Falchetto (CEA) / Dragan Poljak (FESB, University of Split)
11:30	Discussion	
12:30	Lunch Break	
Session 4: Integrated materials/component modelling		
14:00	Introduction	Andrea Sand (VTT)
14:10	Multiscale models for microscopically deformed materials	Sergei Dudarev (UKAEA)
14:50	Dose-dependent fracture toughness prediction: a coupled experimental-numerical approach	Christian Robertson (CEA)
15:30	Coffee Break	
16:00	Bridging the gaps in a multi-scale approach for modelling the effects of irradiation in structural materials: contributions and future perspectives from artificial neural networks	Nicolas Castin (SCK-CEN)
16:40	Materials databases and Calphad	Suzana G. Fries (ICAMS)
17:20	Discussion	
18:20	End	

25th European Fusion Programme Workshop Draft Programme
Dubrovnik, Croatia
Numerical modelling for fusion

Wednesday 29 November 2017

Session 5: Modelling for DEMO and fusion reactors

08:15	Introduction	Matti Coleman (PMU/UKAEA)
08:30	BLUEPRINT, Nova, and advanced integrated DEMO design systems codes	Simon McIntosh (IO/UKAEA)
09:00	Advanced systems codes and integrated modelling for DEMO	Fabrizio Franza (KIT)
09:30	Breeding blanket multi-physics modelling for integrated DEMO design	Alessandro Spagnuolo (KIT)
10:00	Coffee Break	
10:30	Neutronics for systems codes	Jonathan Shimwell (UKAEA)
11:00	Plasma physics modelling for DEMO systems codes	Emiliano Fable (IPP)
11:30	Discussion	
12:30	Lunch Break	

6. Training in Parallel I/O”w systemach i aplikacjach HPC

6.1 Aims

As part of the EoCoE project, Karol Sierociński and Tomasz Paluszkievicz from PSNC (Poznań Supercomputing and Networking Centre) made an internal seminar for PSNC employees, which took place on 17-18 may 2018 at PSNC. The main aim of the course was to show and discuss different parallel I/O strategies using MPI I/O, HDF5, SIONlib, PnetCDF & NetCDF4. 15 people attended this course. Used with the consent of the creators, the materials of the course were created by JSC (Jülich Supercomputing Centre).

6.2 Agenda

N/A.

6.3 Pictures



Figure 4: Pictures of EFPW workshop

6.4 List of participants

Sondage ""Parallel I/O""w systemach i aplikacjach HPC", "

<https://doodle.com/poll/aygqc6axzq4zvuyq>

	Biorę udział
Piotr Szymaniak	OK
Tomasz Piontek	OK
Mirosław Kupczyk	OK
Piotr Śniegowski	OK
Mateusz Matela	OK
Bartek Palak	OK
Daniel Figat	OK
Radosław Januszewski	OK
Rafał Mikołajczak	OK
Marek Błażewicz	OK
Norbert Meyer	OK
Damian Kaliszan	OK
Maciej Brzeźniak	OK
Piotr Brona	OK
Adrian Stelmaszyk	OK
Piotr Kopta	OK
Artur Trojanowski	OK
Nombre	17

1 / 1

6.5 Core metrics of the Workshop

Date: 17-18 of May 2018

Location: PSNC (Poznan, Poland)

Number of registrants: 17

Industrial registrants: 0

Number of attendees: 17

7. EoCoE Workshop in EERA Joint Program

7.1 Aims

In this workshop, the current combined potential of HPC and open source for energy technology modelling have been discussed, formulating a position paper for the creation of a stronger EU position in terms of computational science for energy applications.

The EERA (European Energy research Alliance) Joint Programme on Fuel cells and hydrogen and the IEA (International Energy Agency) Technology Network on Advanced fuel cells are keen to interact with EoCoE to know what opportunities lie in the sharing of resources, computational infrastructure and modelling know-how. Participation of numerical scientists from different energy technology fields (Fuel cells, PV, batteries) helped consolidate an interconnected, open source scientific community for freer and more fertile research.

See the first announcement in appendix for more details.

7.2 Agenda

See agenda here next page.

7.3 Pictures



Figure 5: Pictures Joint Program EoCoE EERA workshop



HIGH PERFORMANCE COMPUTING (HPC) AND OPEN PLATFORMS FOR ENERGY TECHNOLOGY MODELLING

WORKSHOP | PROGRAM

friday, DECEMBER 15th / Royal Continental Hotel, Naples

9:20 > 9:30	Welcome and Opening, scope of the workshop Stephen McPhail, ENEA (Italy)
9:30 > 9:50	The bytes of energy technology modelling HPC for sustainable development data Valeria Jana Schwanitz, HVL (Norway)
9:50 > 10:10	The Energy Oriented Centre of Excellence (EoCoE) Massimo Celino, ENEA (Italy)
10:10 > 10:30	The Open Source Paradigm and CFD modelling Steven Beale, FZJ (Germany)
10:30 > 10:45	A highly scalable finite element framework for complex multiphysics Santiago Badia, UPC (Spain)
10:45 > 11:20	Debate: ICT needs for modelling energy technologies panel of speakers + audience
11:20 > 11:45	Coffee Break
11:45 > 12:00	The physics of energy technology modelling Materials research for energy devices Xavier Granados, ICMAB (Spain)
12:00 > 12:20	Energy storage Thierry Deutsch, CEA (France)
12:20 > 12:40	Multi-scale approaches for fuel cell modelling Mathias Gérard, CEA (France)
12:40 > 13:15	Debate: Common grounds in modelling energy technologies panel of speakers + audience
13:15 > 14:00	Lunch
14:00 > 14:20	The future of energy technology modelling The European Energy Research Alliance: modelling and open source software in the different JPs Holger Ihssen, HZG (Germany)
14:20 > 15:30	Debate: Creating a stronger EU position in terms of computational science for energy applications. Is open source software a way forward ? panel of speakers + audience
15:30	Close of Workshop

7.4 List of participants

See here below the list of participants.

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Figure 6: Participants list of the Joint Program ECoE EERA workshop

7.5 Core metrics of the Workshop

Date: 15 of December 2018

Location: Royal Continental Hotel (Naples, Italy)

Number of registrants: 23

Industrial registrants: 3-4

Number of attendees: 23

See the feedback in appendix.

8. EoCoE-Ampea Workshop

8.1 Aims

The workshop has been jointly organized by EoCoE and AMPEA with the support of EERA. The workshop entitled “New challenges in materials for energy transition: how high performance computing can help to efficient design?” focused the recent game changing developments in the field of materials discovery and design for energy applications boosted by the availability of a new generation of supercomputers and the accessibility of big data collections. There have been 3 scheduled sessions with invited talks and contributed talks and a final round table (4th session).

- Session 1: Accelerating the energy transition: materials meet supercomputers
- Session 2: Accelerating the energy transition: the role of supercomputers
- Session 3: Accelerating the energy transition: the role of materials science
- Session 4: Accelerating the energy transition: strategies to tackle complexity

The workshop has been hold on 7 June 2018 from 09:00-17:00 at the new EERA offices in Brussels. See the application for session in appendix.

8.2 Agenda

See the agenda here next page.

8.3 Pictures



Figure 7: Pictures Joint Program EoCoE Ampea workshop

8.4 List of participants

See the list of participants here below.

Joint EoCoE and AMPEA-EERA workshop

Accelerating the energy transition: challenges in materials design enabled by recent advancements in high performance computing

Date: 7 June 2018

Location: EERA new offices – Rue de Namur 72 - 1000 Brussels – Belgium

		Welcome Coffee	
09:00		Introduction of the workshop	<i>Frédéric Chandezon (CEA, AMPEA) and Massimo Celino (ENEA, EoCoE)</i>
09:05	1.1	Presentation of EERA	<i>Adel El Gammal (EERA)</i>
09:20	S1	Session 1:	
		Accelerating the energy transition (Part 1): materials meet supercomputers	
09:20	1.2	EoCoE: the Energy oriented Centre of Excellence	<i>Edouard Audit (EoCoE, CEA)</i>
09:40	1.3	AMPEA: the EERA Joint Programme and Energy Materials and Processes	<i>Frédéric Chandezon (AMPEA, CEA)</i>
10:00	1.4	EoCoE: the Materials for Energy pillar	<i>Massimo Celino (ENEA, EoCoE)</i>
10:15	1.5	Contributed talk	<i>Marie-Laure Fontaine (SINTEF)</i>
10:30		End of session 1 and coffee break	
11:00	S2	Session 2	
		Accelerating the energy transition (Part 2): the role of supercomputers	
11:00	2.1	EoCoE global HPC support methodology and support activity on Metalwalls	<i>Matthieu Haefele (MdlS, EoCoE)</i>
11:20	2.2	Multiscale modelling of materials, processes and devices in AMPEA	<i>David Lacroix (Lorraine University)</i>
11:40	2.3	Computational characterization of passivating contacts for silicon solar cells	<i>Urs Aeberhard (JFC, EoCoE)</i>
11:55	2.4	Massive MD simulations of an ionic liquid in confinement	<i>Stefano Mossa (CEA Grenoble)</i>
12:10	2.5	Challenges on battery modeling: which tools and methodologies to strengthen the links between atomistic and device simulations	<i>Marion Chandesris (CEA, EoCoE)</i>
12:30		End of session 2 and lunch break	
13:30	S3	Session 3	
		Accelerating the energy transition (Part 3): the role of materials science	
13:30	3.1	EMIRI: the Energy Materials Industrials research Initiative	<i>Simon Perraud (EMIRI)</i>
13:50	3.2	European Energy Materials Development platform	<i>Ihssen Holger (HGF, EERA)</i>
14:10	3.3	Computing with DFT electron transfer effects at interfaces	<i>José C. Conesa (CSIC, Spain)</i>
14:25	3.4	Contributed talk	<i>Tomi Suhonen (VTT)</i>
14:40	3.5	Catalytic Activity of Defective Nanomaterials towards Oxygen Reduction Reaction: An ab initio study	<i>Gracia-Espino Eduardo (Umeå University)</i>
15:00		End of session 3 and coffee break	

15:30	S4	Session 4	
		Accelerating the energy transition (Part 4): strategies to tackle complexity	
15:30	4.1	Mission Innovation. Clean Energy Materials Innovation Challenge 6: to accelerate the exploration, discovery and use of new high performance, low-cost clean energy materials	<i>Monica Fabrizio (CNR, AMPEA) and Ole Martin Løvvik (SINTEF)</i>
15:50	4.2	Round table and general discussion: New challenges in materials for energy transition: how high performance computing can help to efficient design?	
17:00		End of session 4 and end of the event	

		Participation to the Workshop	Participation to the Joint Programme Steering Committee	Email	Signature
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Figure 8: Participants list of the EoCoE-Ampea workshop

8.5 Core metrics of the Workshop

Date: 7th of June 2018

Location: EERA Offices

Number of registrants: 26

Industrial registrants: 1

Number of attendees: 24

9. Hackathon

9.1 Aims

EoCoE in partnership with PRACE PATC and the university of Erlangen organized a three days hackathon on performance engineering. It took place at Maison de la Simulation from June 11th to 13th 2018.

9.2 Agenda

- 1.5 days: lectures on performance engineering methodology
- 1.5 days hands-on: apply the methodology on intensive computing kernels you bring from your code.

9.3 Pictures



Figure 9: Picture of the EoCoE Hackathon

9.4 List of participants

See the list of participants next page.

9.5 Core metrics of the Workshop

Date: 11th - 13th of June 2018

Location: Maison de la Simulation, CEA (Saclay, France).

Number of registrants: 16

Industrial registrants: 0

Number of attendees: 15

10. European Materials Research Society Conference

10.1 Aims

Evolution towards a renewable future demands application-specific materials. Hence, targeted *in silico* searches across chemical space are emerging as critical tools for accelerated materials discovery. This symposium covered all aspects of those efforts, focusing on technologically paramount areas.

We had 142 participants (talks and posters). Among them, 7 invited speakers have attended the Symposium: 2 from USA, 2 from UK, 2 from France, 1 from Spain. Proceedings : selected papers will be published on the international journal “Computational Materials Science” (Elsevier). One phd student has been awarded (450 euro). EoCoE partners were in the scientific committee. EoCoE activities were presented in two talks and several posters. More details are available [here](#).

non-eocoe

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10.2 Agenda

The agenda of the whole Symposium is available in the Appendix.

10.3 Pictures



Figure 10: Picture of the EMRS workshop

10.4 List of participants

See the list of participants here next page.

10.5 Core metrics of the Workshop

Date: 11th - 13th of June 2018

Location: Convention Center, (Strasbourg, France).

Number of registrants: Unknown

Industrial registrants: 6

Number of attendees: 142

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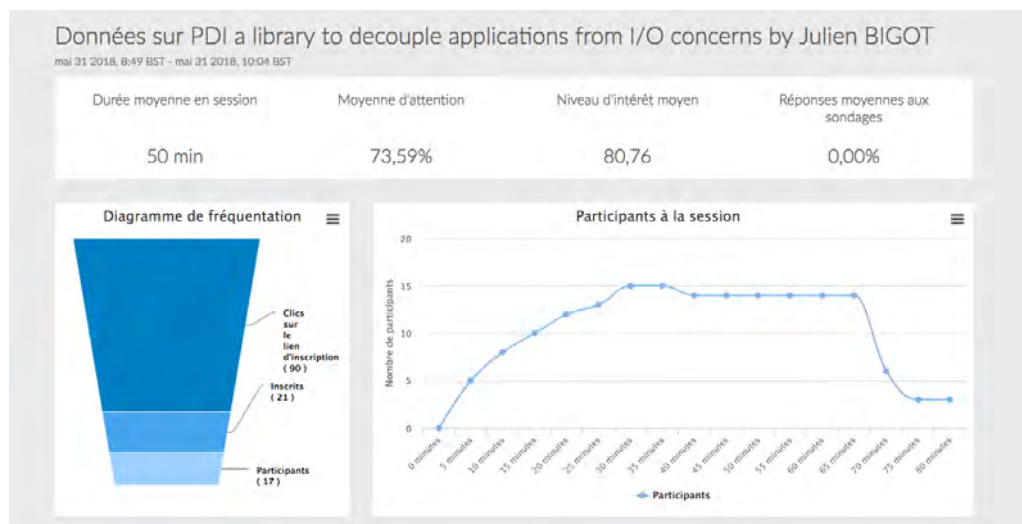
11. EoCoE Webinars

11.1 First EoCoE Webinar: PDI a library to decouple applications from IO concerns.

Speaker: Julien Bigot – Maison de la Simulation – CEA (Saclay)

Abstract: In this talk, I will present the Parallel Data Interface (PDI), a declarative API to decouple application codes from the Input / Output strategy to use. I will present its plugin system that supports the selection of the best suited existing IO library through a configuration file in each part of the code depending on the hardware available, the IO pattern, the problem size, etc. I will demonstrate the advantage of this approach in term of software engineering and performance through the example of the Gysela5D code.

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11.2 Second EoCoE Webinar: Introduction to FPGA computing.

Speaker: Matthieu Haefele (Maison de la Simulation, CNRS)

Abstract: Power budget for supercomputers is already fixed around 20MW. This constraint is already a limiting factor for the current largest petaflop systems and will be a challenging issue for coming exascale computing infrastructures. In this regard, Field Programmable Gate Arrays (FPGA) architectures have a great advantage as their power requirement is roughly one order of magnitude lower than current CPUs. However, as they are streaming devices, the way one has to think to implement numerical simulations is quite different from CPU or even GPU programming. This talk will present FPGA architectures, the way they have to be considered for scientific computing and the Data Flow Engine (DFE) programming model proposed by Maxeler.

Rapport participation

PDI a library to decouple applications from I/O concerns by Julien BIGOT

Rapport généré :

13/09/18 14:43 BST

Identifiant du webinaire	Date et heure de début actuelles	Durée	Nb inscrits	Nb participants	Clics sur le lien d'inscription
150-214-891	31/05/18 9:49 CEST	1 heure 16 minutes	21	17	90

Détails du participant

Participé	Taux d'intérêt	Nom	Prénom	Adresse e-mail	Durée de session
Oui	97	Ahmed	Aqeel	ahmeda@coria.fr	54 minutes
Oui	46	Celino	Massimo	massimo.celino@enea.it	52 minutes
Oui	99	Delande	Dominique	Dominique.Delande@lkb.upmc.fr	1 heure 8 minutes
Oui	97	Delorme	Maxime	m.delorme@surrey.ac.uk	55 minutes
Oui	95	Digonnet	Hugues	hugues.digonnet@ec-nantes.fr	38 minutes
Oui	90	Funel	Agostino	agostino.funel@enea.it	57 minutes
Oui	64	Gibbon	Paul	p.gibbon@fz-juelich.de	21 minutes
Oui	100	Haefele	Matthieu	Matthieu.HAEFELE@cea.fr	1 heure 16 minutes
Oui	38	Kirkos	George	g.kirkos@cyi.ac.cy	47 minutes
Oui	99	Lemesios	Christos	c.lemesios@cyi.ac.cy	1 heure 11 minutes
Oui	44	Martin	Benoit	benoit.martin@inria.fr	28 minutes
Oui	71	Nicolas	Timothee	timothee.nicolas@gmail.com	49 minutes
Oui	97	Parsons	David	david.parsons@inria.fr	56 minutes
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Oui	99	Torun	Fahreddin Sukru	ftorun@enseeiht.fr	1 heure 6 minutes
Oui	98	Wautelet	Philippe	philippe.wautelet@aero.obs-mip.fr	1 heure 1 minute
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Rapport

participation :

Rapport généré :

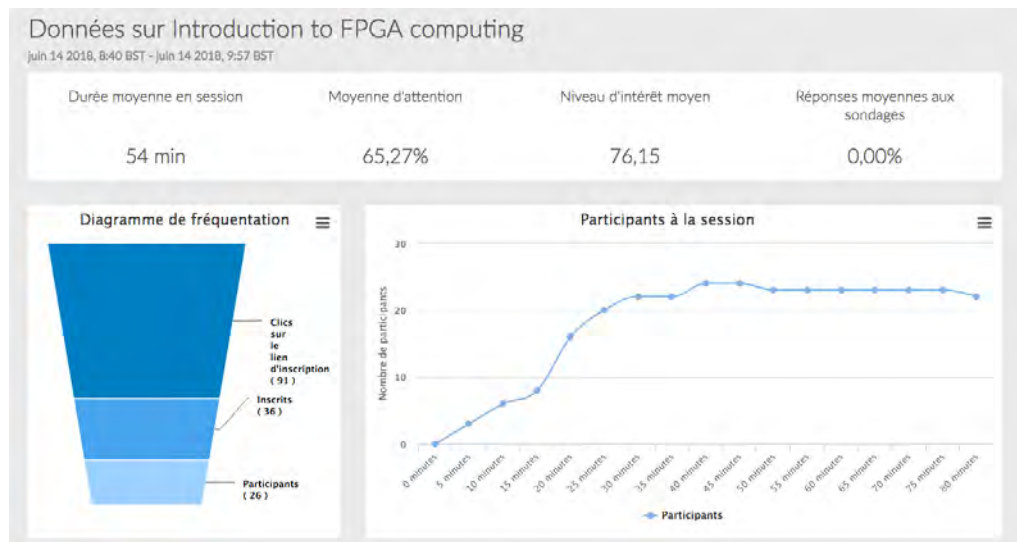
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Identifiant du webinaire	Date et heure de début actuelles	Durée	Nb inscrits	Nb participants	Clics sur le lien d'inscription
474-979-347	14/06/18 9:40 CEST	1 heure 17 minutes	36	26	91

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Oui	69	Funel	Agostino	agostino.funel@enea.it	57 minutes
Oui	39	Grandgirard	Virginie	virginie.grandgirard@cea.fr	1 heure 1 minute
Oui	93	HAEFELE	Cécile	cecile.haeefe@gmail.com	25 minutes
Oui	99	Haefele	Matthieu	Matthieu.HAEFELE@cea.fr	1 heure 6 minutes
Oui	99	Hagemeier	Annika	a.hagemeier@fz-juelich.de	1 heure 8 minutes
Oui	98	Halver	Rene	r.halver@fz-juelich.de	1 heure 2 minutes
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Oui	45	Pérignon	Franck	Franck.Perignon@univ-grenoble-alpes.fr	48 minutes
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Oui	98	Soni	Vineet	vineet.soni@cea.fr	60 minutes
Oui	41	Staffelbach	Gabriel	gabriel.staffelbach@cerfacs.fr	41 minutes
Oui	100	Suckert	Rene	jensrene.suckert@uni-jena.de	1 heure 15 minutes
Oui	90	Sutmann	Godehard	g.sutmann@fz-juelich.de	3 minutes
Oui	100	Vanzo	Daniel	daniel.vanzo@lri.fr	1 heure 17 minutes
Oui	98	Vulpescu	Bogdan	bogdan.vulpescu@clermont.in2p3.fr	59 minutes
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Oui	98	delamare	simon	simon.delamare@ens-lyon.fr	60 minutes
Oui	53	farjallah	asma	asma.farjallah@intel.com	11 minutes
Oui	66	marradi	luca	lucamarradi@yahoo.it	1 heure 3 minutes
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11.3 Third EoCoE Webinar: Perovskite materials for solar cells: atomic-scale insights from ab initio modelling.

Speaker: Dibyajyoti Ghosh (Department of Physics & Department of Chemistry, University of Bath, Bath BA2 7AY, U.K.).

Abstract: Metal halide perovskite solar cells have rapidly emerged as leading contenders in photovoltaic technology. However, the poor structural stability and toxicity related to lead seriously hinder the advancement of this field. Compositional engineering is found to be the promising solution to these challenges. In this talk, atomic-scale insights into the local structures and dynamics of mixed A-cation compositions based on formamidinium lead iodide ($\text{CH}(\text{NH}_2)_2\text{PbI}_3$) doped with Cs^+ , Rb^+ and MA^+ will be first discussed. These compositions show the best performance and have higher stability in the family of hybrid perovskite materials.[1] Our specific findings include the first indication that substitution of low concentrations of smaller cations on the A-site in $\text{CH}(\text{NH}_2)_2\text{PbI}_3$ results in a global ‘locking’ of the PbI_6 octahedra tilting and reduced lattice dynamics. A key impact of this feature is that the rotational or tumbling motion of the $\text{CH}(\text{NH}_2)_2^+$ molecular ion in a locked cage is severely restricted. We discuss the impact of locking on the photovoltaic performance and stability. The second part of the talk will be focused on the use of tin and germanium as possible replacements of lead. The tin and germanium-based perovskites are thermodynamically stable and exhibit promising optical properties.[2] These studies help the community to gain a fundamental understanding of composition engineering of hybrid perovskites. 1. Ghosh et al. ACS Energy Lett. 2017, 2, 2424 2. Nagane et al. J. Phys. Chem. C, 2018, 122, 5940

Rapport participation :

Perovskite materials for solar cells: atomic-scale insights from ab initio modelling

Rapport généré :

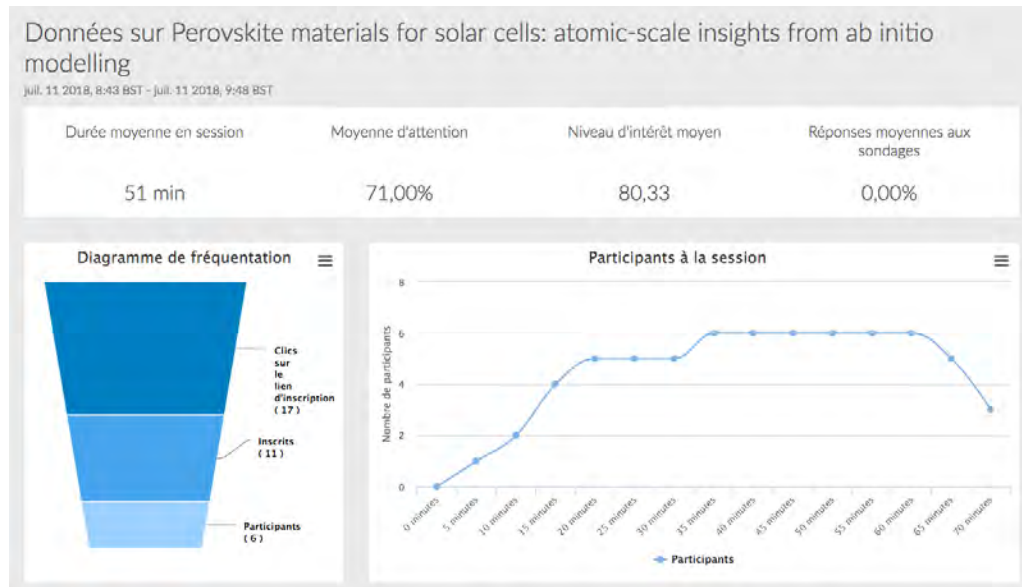
13/09/18 14:45 BST

Identifiant du webinaire	Date et heure de début actuelles	Durée	Nb inscrits	Nb participants	Clics sur le lien d'inscription
345-970-211	11/07/18 9:43 CEST	1 heure 6 minutes	11	6	17

Détails du participant

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Oui	82	Emiliano	Burresi	emiliano.burresi@enea.it	33 minutes
Oui	72	Francesco	Buonocore	francesco.buonocore@enea.it	54 minutes
Oui	99	Ghosh	Dibyajyoti	dg617@bath.ac.uk	57 minutes
Oui	96	Gusso	Michele	michele.gusso@enea.it	52 minutes
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11.4 Fourth EoCoE Webinar: An introduction to ensemble simulations and data assimilation in the context of high performance scientific computing.

Speaker: Harrie-Jan Hendricks-Franssen (Forschungszentrum Jülich GmbH).

Abstract: Whereas high-performance scientific computing in the 90's of the 20th century focused mostly on forward single-physics problems, using parallel computing, the 21st century has seen a shift towards multi-physics problems, ensemble simulations and massively parallel computing. Recently the focus towards data-driven modelling has been re-enforced. In this context, this webinar will discuss different approaches for data driven modelling relevant for simulation models based on the numerical solution of partial differential equations (PDE). The webinar will give an overview on different data-driven modelling techniques like (i) inverse modelling or variational data assimilation, (ii) sequential data assimilation (Ensemble Kalman Filter variants and Particle Filters), and (iii) Markov Chain Monte Carlo techniques. In addition, an outlook will be given on the potential role of machine learning for PDE-based model-data fusion techniques.

Rapport participation :

Rapport généré :
13/09/18 14:42 BST

An introduction to ensemble simulations and data assimilation in the context of high performance scientific computing

Identifiant du webinaire	Date et heure de début actuelles	Durée	Nb inscrits	Nb participants	Clics sur le lien d'inscription
311-464-971	11/09/18 9:34 CEST	1 heure 49 minutes	70	43	141

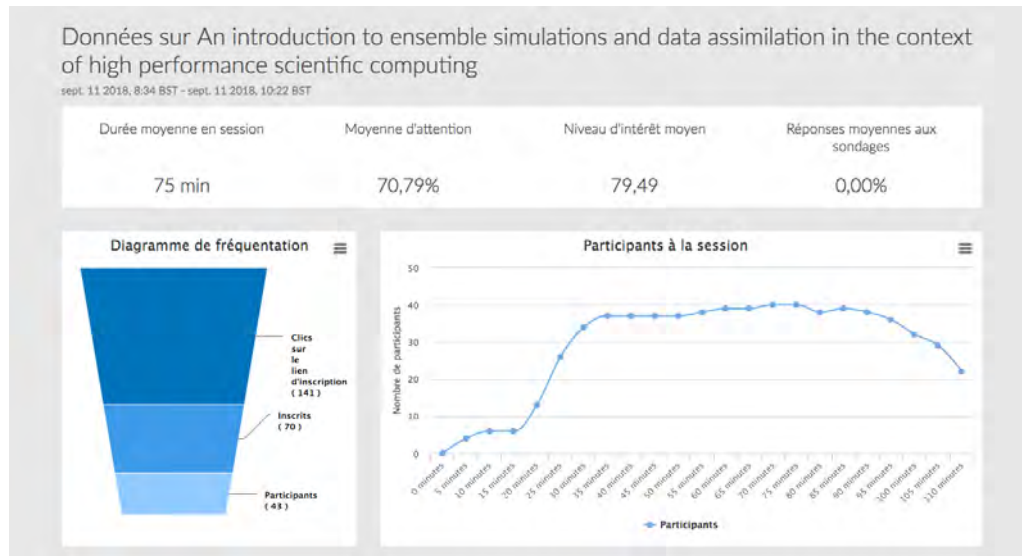
Détails du participant

Participé	Taux d'intérêt	Nom	Prénom	Adresse e-mail	Durée de session
Oui	62	Aillaud	Pierre	pierre.aillaud.1@gmail.com	1 heure 18 minutes
Oui	64	Baumeister	Paul	p.baumeister@fz-juelich.de	1 heure 24 minutes
Oui	83	Bauser	Hannes	hannes.bauser@iup.uni-heidelberg.de	1 heure 31 minutes
Oui	50	Besombes	Camille	besombescamille@hotmail.fr	1 heure 14 minutes
Oui	86	Büsing	Henrik	hbuesing@eonerc.rwth-aachen.de	1 heure 33 minutes
Oui	98	Christoudias	Theodoros	christoudias@cyi.ac.cy	1 heure 25 minutes
Oui	75	Comito	Claudia	c.comito@fz-juelich.de	1 heure 20 minutes
Oui	44	D'Ambra	Pasqua	pasqua.dambra@cnr.it	1 heure 9 minutes
Oui	99	DUPAYS	ISABELLE	isabelle.dupays@idris.fr	1 heure 36 minutes
Oui	95	Dal Molin	Marco	marco.dalmolin@eawag.ch	59 minutes
Oui	95	Dayal	Deen	deemishra26@gmail.com	51 minutes
Oui	93	Deb Barma	Surajit	surajitdb@gmail.com	1 heure 30 minutes
Oui	100	Figura	Clarissa	clarissa.figura@uni-bonn.de	1 heure 48 minutes
Oui	98	Finkenrath	Jacob	j.finkenrath@cyi.ac.cy	1 heure 29 minutes
Oui	42	Gibbon	Paul	p.gibbon@fz-juelich.de	1 heure 24 minutes
Oui	98	Goergen	Klaus	k.goergen@fz-juelich.de	1 heure 25 minutes
Oui	43	Gonzalez-Nicolas	Ana	ana.gonzalez@iws.uni-stuttgart.de	1 heure 24 minutes
Oui	97	HECTOR	Basile	basile.hector@ird.fr	1 heure 17 minutes
Oui	97	Haefele	Matthieu	Matthieu.HAEFELE@cea.fr	1 heure 21 minutes
Oui	100	Koh	Seong-Ryong	s.koh@fz-juelich.de	1 heure 45 minutes
Oui	98	Kolberg	Sjur	Sjur.Kolberg@enki-hydrologi.no	1 heure 22 minutes
Oui	42	Kurzrock	Frederik	frederik.kurzrock@reuniwatt.com	1 heure 12 minutes
Oui	98	Lauvernet	Claire	claire.lauvernet@irstea.fr	1 heure 25 minutes
Oui	98	Leblois	Etienne	etienne.leblois@irstea.fr	1 heure 27 minutes
Oui	98	Mai	Trung Hieu	mai.trunghieu@yahoo.com	1 heure 25 minutes

Oui	39	Mayo-García	Rafael	rafael.mayo@ciemat.es	1 heure 17 minutes
Oui	81	Mirouze	Isabelle	isabelle.mirouze@cerfacs.fr	54 minutes
Oui	59	Naz	Bibi	b.naz@fz-juelich.de	1 heure 20 minutes
Oui	89	Nguyen	Hiep	moitruong178@gmail.com	1 heure 30 minutes
Oui	68	Nguyen	Quan	quannguyen201294@gmail.com	1 heure 15 minutes
Oui	90	Nikolaou	Zacharias	z.nicolaou@cyi.ac.cy	2 minutes
Oui	98	Ouyang	Bingjie	bingjie.ouyang.gr@dartmouth.edu	1 heure 23 minutes
Oui	93	PARIENTE	FREDERIC	fpariente@nvidia.com	1 heure 12 minutes
Oui	98	Piacentini	Andrea	piacentini.palm@gmail.com	1 heure 22 minutes
Oui	68	Queloz	Pierre	pierre.queloz@heig-vd.ch	1 heure 29 minutes
Oui	41	RAFFIN	Bruno	bruno.raffin@inria.fr	1 heure 28 minutes
Oui	75	Sawicz	Keith	ksawicz@air-worldwide.com	5 minutes
Oui	98	Schuster	Dominik	schuster@cerfacs.fr	1 heure 26 minutes
Oui	41	Silva	Luisa	luisa.alexandra.silva87@gmail.com	1 heure 47 minutes
Oui	90	TORUN	Fahreddin Sukru	fsukrutorun@gmail.com	6 minutes
Oui	98	Terraz	Théophile	theophile.terraz@inria.fr	1 heure 31 minutes
Oui	47	Walker	Alison	a.b.walker@bath.ac.uk	1 heure 9 minutes
Oui	92	Wright	David	dave.wright@ucl.ac.uk	23 minutes
Non	0	Ali	Javed	javedali28@gmail.com	--
Non	0	Anurag	Harsh	anura003@umn.edu	--
Non	0	Berndt	Jonas	j.berndt@fz-juelich.de	--
Non	0	Chinnayakanahalli	Kiran	kchinnayakanahalli@air-worldwide.com	--
Non	0	Dars	Ghulam	darsghulam@gmail.com	--
Non	0	Ding	Junyan	djunyan@ucalgary.ca	--
Non	0	Dwivedi	Dipankar	ddwivedi@lbl.gov	--
Non	0	Hosseini	Atefeh	ahosseini786@gmail.com	--
Non	0	Huang	Suilou	shuang@air-worldwide.com	--
Non	0	Jarihani	Ben	bjarihan@usc.edu.au	--
Non	0	Keune	Jessica	jessica.keune@ugent.be	--
Non	0	Kim	Jongho	jhjheheh@gmail.com	--
Non	0	Li	Xueke	xueke.li@uconn.edu	--
Non	0	Masafu	Christopher	masafu@gmail.com	--
Non	0	Mehan	Sushant	smehan@purdue.edu	--
Non	0	Montes	Felipe	frm10@psu.edu	--
Non	0	Osores	Soledad	msosores@smn.gob.ar	--
Non	0	Portella	Felipe	felipe@portella.com.br	--

Non	0	RANDRIATOAMANANA	RICHARD	richard.randriatoamanana@ec-nantes.fr	--
Non	0	Rahi	Nazim Uddin	rahicox@gmail.com	--
Non	0	S	Niranjana	niranjana.am16f05@nitk.edu.in	--
Non	0	Singh	Amit	mail.amsingh5@gmail.com	--
Non	0	Son	Kyongho	kkyong77@hotmail.com	--
Non	0	Tang	Darrell	darrell.tang@wur.nl	--
Non	0	Winter	Kevin	kevin.winter@iee.fraunhofer.de	--
Non	0	Zaman	Badruz	badruz@rpm-engineers.com.my	--
Non	0	bane	michael	mkb@highendcompute.co.uk	--

Metrics



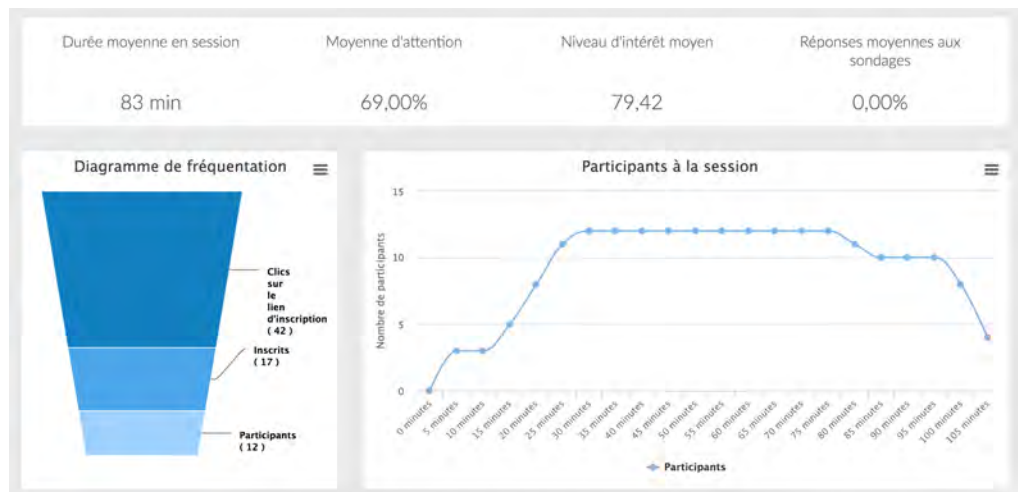
11.5 Fifth EoCoE Webinar: HPC Modelling of Turbulent Transport in Tokamak Plasmas: Recent Results regarding Critical Physical Issues.

Speaker: Yanick Sarazin (CEA)

Abstract: Turbulence governs heat confinement in tokamak fusion plasmas. In turn, turbulence properties explain why large machines, like ITER, are required so as to reach the desired performance in terms of energy gain. Understanding, predicting and possibly controlling turbulent transport is therefore of outermost importance in fusion research. In addition to experimental measurements, High Performance Computing (HPC) now allows one to gain much insight in these critical issues. The talk will first recall the basic principles of controlled fusion and of plasma confinement in tokamaks. The main features of turbulence and transport will be reviewed, with implications on the required modelling effort. The focus will be put on turbulence self-organization and on the multi-scale aspect of the problem, in particular regarding the interaction between electron and ion scales on the one hand, and ion and equilibrium scales on the other hand. The role of sheared flows will be shown to be critical. Finally, the route towards turbulence control will be discussed, emphasizing the modelling effort of the spontaneous bifurcation to transport barriers characterized by improved confinement regimes.

See participants report next page.

Metrics



12. Final EoCoE Conference in Cyprus

See deliverable D6.15.

Rapport participation :

Rapport généré :

26/09/18 10:20 BST

Identifiant du

webinaire	Date et heure de début actuelles	Durée	Nb inscrits	Nb participants	Clics sur le lien d'inscription
417-552-931	25/09/18 10:40 CEST	1 heure 44 minutes	17	12	42

Détails du participant

Participé	Taux d'intérêt	Nom	Prénom	Adresse e-mail	Durée de session
Oui	89	Albert Devasagayam	Francis Clinton Prasanth	francisclinton93@gmail.com	1 heure 40 minutes
Oui	97	Biancalani	Alessandro	biancalani@ipp.mpg.de	1 heure 22 minutes
Oui	62	Body	Thomas	thomas.body@ipp.mpg.de	1 heure 15 minutes
Oui	98	Broemmel	Dirk	d.broemmel@fz-juelich.de	1 heure 22 minutes
Oui	95	Chew	Junxian	j.chew@fz-juelich.de	1 heure 17 minutes
Oui	100	Finkenrath	Jacob	j.finkenrath@cyi.ac.cy	1 heure 42 minutes
Oui	40	Gibbon	Paul	p.gibbon@fz-juelich.de	1 heure 24 minutes
Oui	49	Jony	Castagna	jony.castagna@stfc.ac.uk	57 minutes
Oui	98	Lips	Johannes	johannes.lips@hotmail.com	1 heure 26 minutes
Oui	88	Somers	Robin	robin.somers@ugent.be	1 heure 30 minutes
Oui	39	TORUN	Fahreddin Sukru	fsukrutorun@gmail.com	1 heure 9 minutes
Oui	98	Zholobenko	Wladimir	wlz@ipp.mpg.de	1 heure 36 minutes
Non	0	Devitre	Alexis	alexisrdevitre@gmail.com	--
Non	0	Luk	Onnie	onnie.luk@ipp.mpg.de	--
Non	0	Sytova	Elizaveta	elizavetasytova@gmail.com	--
Non	0	Unaldi	Selen	selennald@gmail.com	--
Non	0	cutillas	jose manuel	gyrox_x@hotmail.com	--

A. APPENDIX

SYMPOSIUM B

Theoretical searches for innovative materials
for energy harvesting and storage

Symposium Organizers :

Jesús CARRETE MONTAÑA , TU Wien, Austria

Massimo CELINO, ENEA, Roma, Italy

Natalio MINGO, CEA Grenoble, France

To be published in Computational Materials Science, Elsevier

Supported by the European Energy oriented Centre of Excellence (EoCoE),
grant agreement number 676629, funded within the Horizon2020
framework of the European Union.



08:30 **INV** **B 4.1** **Network glasses for innovation in applied science: fundamental issues and new insights.**

Carlo Massobrio
Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, F-67034 Strasbourg, France

09:00 **B 4.2** **Good Vibrations: Locking of Octahedral Tilting in Mixed-Cation Iodide Perovskites for Solar Cells**

Dibyayoti Ghosh,† Philip Walsh Atkins,† M. Salih Islam,*, ‡ Alison B. Walker,*, † and Christopher Eames,†
†Department of Physics, University of Bath, Bath BA2 7AY, U.K. ‡Department of Chemistry, University of Bath, Bath BA2 7AY, U.K.

09:15 **B 4.3** **High throughput search for high mobility p-type transparent conducting materials: identification of BP, Cate and L035b**

V.-A. Ha, G. Yu, F. Ricci, M. J. van Setten, M. Giamtomassi, G.-M. Rignanese and G. Hautier
Condensed Matter and Nanoscience (IMCN), Université catholique de Louvain (UCL), Chemin éolies 8, bte L7.03.01, Louvain-la-Neuve 1348, Belgium

09:30 **B 4.4** **Simulative study on the effect of ferroelectric domains in perovskite solar cells**

Daniele Rossi, Matthias Auf der Maur, Alessandro Pecchia, Aldo Di Carlo
Dipartimento di Ingegneria Elettronica, Università di Tor Vergata, Rome, Italy, Dipartimento di Ingegneria Elettronica, Università di Tor Vergata, Rome, Italy, Istituto per lo Studio dei Materiali Nanostrutturati (ISMN), Consiglio Nazionale delle Ricerche (CNR), Rome, Italy, Dipartimento di Ingegneria Elettronica, Università di Tor Vergata, Rome, Italy.

09:45 **B 4.5** **Fluctuations in Pristine Hybrid Perovskite Systems from First Principles Methods**

Marcelo A. Caigiano, Jacky Even, Claudine Katan
Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, P.O. Box 14110, Doha, Qatar, Univ Rennes, INSA Rennes, CNRS, Institut FOTON - UMR 6082, F-35000 Rennes, France, Univ Rennes, ENSCR, INSA Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226, F-35000 Rennes, France.

10:00 **B 5.1** **Coffee Break**

Photovoltaic and Optical Materials (III) : C. Massobrio

10:30 **INV** **B 5.1** **Physics of multilayered halide perovskite semiconductors**

J. Even, H. Tsai, W. Nie, J.-C. Blancon, A. Neukirch, L. Pedesseau, B. Traoré, M. Kepenekian, C. Stoumpos, M. Stier, J. Crochet, S. Tretiak, M. Kanatzidis, A. Mohite, C. Katan
FOTON, UMR 6082, CNRS, INSA Rennes, Rennes, France, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, FOTON, UMR 6082, CNRS, INSA Rennes, Rennes, France, ISCR, UMR 6226, CNRS, Université de Rennes 1, Rennes, France, Department of Chemistry, Northwestern University, Evanston, Illinois USA, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, USA, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, Department of Chemistry, Northwestern University, Evanston, Illinois USA, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, ISCR, UMR 6226, CNRS, Université de Rennes 1, Rennes, France.

11:00 **B 5.2** **Optoelectronic properties of GaNAsBi/GaAs strained structures**

W. Q. Jemmal†, N. Anef, M. M. Habbchi, A. Rebey
University of Monastir, Faculty of sciences, Unité de Recherche sur les Hétéro-Epitaixes et Applications / Corresponding author : winedjemmal@gmail.com

11:15 **B 5.3** **Understanding relations between structural effects and electronic properties in CH3NH3PbI3 perovskite**

Propin (c), J. C. Conesa (c)
(a) Instituto de Energía Solar and Dept. TF6, E.T.S.I. Telecomunicación
(b) Instituto Politécnico de Madrid, Spain, (c) Instituto de Energía Solar and Dept. FANAE, Universidad Carlos III de Madrid, Spain, (d) Instituto de Física, (e) Departamento de Física, Facultad de Ciencias, Universidad de Chile, Chile, (d) Instituto de Catálisis y Petroleoquímica, CSIC, Marie Curie 2, Madrid, Spain.

11:30 **B 5.4** **Phenomenological modelling of light transmission through narrowvires arrays**

J. Zhour, L. O. Le Curif, K. Nomenjo, A. Viat, T. Papiorek and G. Lerondell
Laboratoire d'Optique Photonique et Photonique Quantique, Institut Charles Delaunay, CNRS UMR 8281, Université de Technologie de Compiègne, 12 rue Marie Curie, CS 42060, 10004 Troyes Cedex France, 2. Chimie Paritech, PSI Research University, CNRS, Institut de Recherche de Chimie Paris (IRCP), 11 rue Pierre et Marie Curie, 75005 Paris, France

11:45 **B 5.5** **Exact analytical expressions of photovoltaic module physical parameters modelling effects of incident irradiance and temperature**

El Mahdi ASSAID, Hicham EL ACHOUY, Mhamed ZAIMI, Asmaa IBRAH, Safae AZOU
Optics and Electronics of Semiconductor Nanostructures Team, Department of Physics, Faculty of Sciences, Chouato Doukkali University, Moroccan Foundation for Advanced Sciences, Innovation and Research (MASRI), Optics and Photonics Center, Rabat, Morocco

12:30 **B 6.1** **Lunch Break**

Cathode Materials : J. Even

14:00 **INV** **B 6.1** **Materials Design of High-Energy Cation/Anion Redox in Li-rich Cathode Materials**

Chris Wolverton
Northwestern University, Dept. of Materials Science and Eng.

14:30 **B 6.2** **Transport of Na in Na_xFePO₄ cathode material: Insights from advanced force-field Molecular Simulations**

Mauricio R. Bonilla (1), Ariel Lozano (2), Bruno Escribano (1), Javier Carrasco (3), Elena Akhmetkayeva (1,4)
1- Basque Center for Applied Mathematics, Alameda de Mazarredo 14 (48009) Bilbao, Spain; 2- Materials Institute, University of Liège, Allée du Sautourverte, 4000, Sart Tilman, Belgium; 3- Centre for Energy Storage, 48105 (10) Madrid, Spain; 4- KERBASQUE, Basque Foundation for Science (48013) Bilbao, Spain

14:45 **B 6.3** **Computational search for new stable reconstruction of the (110) surface of RuO₂ and its role in pseudocapacitance**

Hayk A. Zakaryan, Alexander G. Kvashnin, Artem R. Oganov
Yerevan State University, Skolkovo Institute of Science and Technology, Moscow Institute of Physics and Technology, Northwestern Polytechnical University

15:00 **B 6.4** **Using Cluster Expansion to Characterize Battery Cathode Materials: Implications for Application**

Jin Hyun Chang, Juan Maria Garcia-Lastra, Teis Vegge
Department of Energy Conversion and Storage, Technical University of Denmark, Department of Energy Conversion and Storage, Technical University of Denmark, Department of Energy Conversion and Storage, Technical University of Denmark

15:15 **B 6.5** **Structural Characterization of the Li-Ion Battery Cathode Materials LiT_{0.5}Mn_{2-x}O₄ (0.2 ≤ x ≤ 1.5) with 7Li NMR and DFT**

Roberta Pigliapochi, Itean Seymour, Céline Merlet, Andrew Pelli, Denissa Murphy, Siebert Schmid, Claire Grey
Department of Chemistry, University of Cambridge, School of Chemistry, University of Sydney

15:30 **B 7.1** **Coffee Break**

Anode Materials : C. Wolverton

16:00 **B 7.1** **VS₂/Graphene Heterostructures as Promising Anode Material for Li-Ion Batteries**

Zakhar I. Popov, Maxim A. Vozin, Natalia S. Mikhaleva
National University of Science and Technology, MISIS, 4 Leninsky prospekt, Moscow, 119049, Russian Federation, Siberian Federal University, 79 Svyobodny av., Krasnoyarsk, 660041, Russian Federation, Kirensky Institute of Physics, 5038 Akademgorodok, Krasnoyarsk, 660036, Russian Federation

16:15 **B 7.2** **The Role of Solvent in Intercalation of Sodium Ion into Graphite from Quantum Mechanics to Molecular Dynamics Simulations**

Al Kachmar, William A. Goddard III
Qatar Environment and Energy Research Institute, Hamed Bin Khalifa University, Omsiyah, Doha, Qatar, Materials and Process Simulation Center, University of California Institute of Technology, Pasadena, California 9125, United States

16:30 **First-principles Investigation of 2D Materials in Lithium Ion battery and photocatalytic CO₂ decomposition** **B 7.3**
 Tianhui Wang, Yanyan Song, Kang
 Institute for Application of Advanced Materials, Jeonju University, SOUTH KOREA
 Department of Nano & Advanced Materials, Jeonju University, SOUTH KOREA

16:45 **First-Principles Study of Sodium Intercalation in Crystalline NaxS₂ (0 ≤ x <= 4) as Anode Material for Na-ion Batteries** **B 7.4**
 Oier Arceles Unai Arrieta, Nebil A. Katcho, Javier Carrasco
 CIC Energigune

17:00 **An Ab-initio Study of Lithiated SnO₂ as Anode Material for Li-ion Batteries** **B 7.5**
 Omerik Baskin, Tomáš Buncák, Mathias Jansen
 Integrated Systems Laboratory, Department of Information Technology and Electrical Engineering, ETH Zürich, Gloriastrasse 35, 8092 Zürich, Switzerland

B-10

Wednesday 20 June 2018

Thermoelectrics and Thermal Storage (I) : I. Savic

08:30 INV Advanced materials in Energy harvesting and storage in IK4-TEKNIKER **B 8.1**
 A. Igaruta, B. Coto, J. Barriga, E. Aranzabe
 IK4-TEKNIKER

09:00 Multiscale modelling tools for solar thermal energy collection and storage **B 8.2**
 Annalisa Cardellini, Matteo Abergini, Matteo Fasano, Edoardo Chivazzo, Pietro Pollicino di Torino

09:15 Pressure-induced conduction band convergence in the thermoelectric ternary chalcogenide CuBS₂ **B 8.3**
 Najebah M. Alsaieh, Elvis Shoko, and Udo Schwingenschlgl
 King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

09:30 Thermal conductivity of cubic vs hexagonal semiconductors from first-principles **B 8.4**
 Riccardo Rurali, Marti Raya-Moreno, Hugo Aramberri, Juan Antonio Seijas-Bellido, Xavier Cardóka
 Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus de Bellaterra, 08193 Bellaterra, Barcelona, Spain, Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona, Spain

09:45 Calculating Transport Properties Using the DFT Method and Boltzmann Approach: Application to Mg₂Sb_{1-x}Sn_x Thermoelectrics **B 8.5**
 Brahim MARHOUCHE 1/ Hamza LIDJICHI 1, 3, / Brahim LAGOUN 2, / Pascal Boulet 4, / Marie-Christine Record 5
 1: Laboratoire GREMAH de développement des matériaux semi-conducteurs et des matériaux thermoelectriques, Université de Chlef, Route de Ghazal, B.P. 373, Algérie, 2: Laboratoire de physique des matériaux, Université de Laghouat, Algérie, 3: Laboratoire de physique des matériaux, Université de Laghouat, Route de Ghazal, B.P. 753, Laghouat, Algérie, 4: Laboratoire des Matériaux et Procédés, Université de Valenciennes et du Hainaut-Cambrésis, 2,1 du Champ de l'Abbesse 59600 Maubeuge, France, 5: MADIREL, Aix-Marseille University and CNRS, Avenue Normandie-Niemen, 13397 Marseille cedex 20, France, 5: IM2NP, Aix-Marseille University and CNRS, Avenue Normandie-Niemen, 13397 Marseille cedex 20, France.

10:00 Coffee Break

Thermoelectrics and Thermal Storage (II) : A. Igaruta

10:30 INV Role of entropy in finding new materials **B 9.1**
 Stefano Curtarolo
 Duke University USA, Fritz-Haber Institute, Berlin, Germany

11:00 Intrinsic phonon-limited charge carrier mobilities in thermoelectric SnSe **B 9.2**
 Wu Li, Jinlong Ma
 Shenzhen University, China

11:15 Electron-phonon coupling and thermoelectric transport in n-type PbTe. **B 9.3**
 J.D. Querales-Flores (1), J. Cao (1), R. Murphy (1,2), S. Fahy (1,2) and I. Savic (1).
 (1) Tyndall National Institute, Cork, Ireland. (2) University College Cork, Cork, Ireland.

11:30 Role of force-constant disorder in the lattice thermal conductivity of thermoelectric materials **B 9.4**
 Marco Arigioli, Jesús Carrete, Natalio Mingo, Georg K. H. Madsen
 Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria
 Materials Chemistry, TU Wien, A-1060 Vienna, Austria, CEA, LITEN, 17 rue des Martyrs, F-38054 Grenoble, France, Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria

11:45 Assessment of thermoelectric performance of half-Heusler materials: GW, HSE and DFT methods compared **B 9.5**
 Peter Kratzer and Maedeh Zarehdar
 Faculty of Physics, University of Duisburg-Essen

12:00 Lunch Break

B-11

14:00	Silica nanoparticles-ionic liquid composites electrolyte for energy storage devices Hyun Young Jung, Sung Mi Jung Gyeongnam National University of Science and Technology, Korea Institute of Toxicology	B P2.1	14:00	Controllable Structure Transitions of Mn₃O₄ Nanomaterials and Their Effects on Electrochemical Properties Jing Wang, Jingdong Cai, John Wang Department of Materials Science & Engineering, National University of Singapore, 9 Engineering Drive 1, 117576, Singapore, b. Institute of Materials Research and Engineering, A*STAR (Agency for Science, Technology and Research), 2 Fusionopolis Way, Innovis, Singapore 138634, c. Institute of High Performance Computing, A*Star (Agency for Science, Technology and Research), 1 Fusionopolis Way, Connexis, Singapore 138632	B P2.13
14:00	Temperature reduction of c-Si solar cell using transparent multilayer passive radiative cooling stack Avinash Kumar, Anariya Chowdhury Centre for Energy and Environment, J.L.N. Marg, Jaipur, India -302 017	B P2.2	14:00	Probing the ferroelectric nature of the tetragonal phase of CH₃NH₃PbI₃ with ab initio molecular dynamics Ioannis Deretzis 1), Antonino La Magna 1) 1) CNR-IMM Zona Industriale VIII Strada 51 95121	B P2.15
14:00	High-performance Si-based anode material synthesized by the combination of phosphorus and CNT Byung Hoon Park, Kwang Bum Kim Department of Materials Science and Engineering, Yonsei University	B P2.3	14:00	Ab initio stability of hydroxylated graphene Francesco Buoncore (a), Andrea Capasso (b), Nicola Lisi (a) (a) ENEA, Casaccia Research Centre, I-00123 Rome, Italy, (b) Istituto Italiano di Tecnologia, Graphene Labs, Via Morego 30, Genova 16163, Italy	B P2.16
14:00	SIP2/CNT composite as a promising anode material for high-performance Li-ion batteries Byung Hoon Park, Kwang Bum Kim Department of Materials Science and Engineering, Yonsei University	B P2.4	14:00	Built in electric field effects on the conversion efficiency in intermediate band solar cells. A. EL Aouami (a), M. El Hachimi (a,b), M. EL-Yadiri (a), E. Feddi (a,b) and F. Alardj (c) (a) Laboratoire d'optoelectronique des boites quantiques des semiconducteurs, ENSSET, Meiraneq V University in Rabat, Morocco, (b) Centre Regional des Metiers de l'Education et de Formation (CRMEF), Tanger, Tetouan, (c) LCP-A2MC, Institut de Chimie, Physique et Matériaux Université de Lorraine, Metz, France,	B P2.17
14:00	Study of Potassium Ion Storage Mechanism in Anatase TiO₂ Anode Material for Rechargeable Batteries Geon-Woo Lee, Young-Hwan Kim, Ha-Kyung Roh, Byung Hun Park, Kwang Bum Kim Department of Materials Science and Engineering, Yonsei University, 134 Shinchon-Dong, Seodaemun-gu, Seoul 120-749, Republic of Korea	B P2.5	14:00	The effect of organic solvent additive in ionic liquid on rechargeable aluminum-ion battery Danbi Lee, Youngho Oh, Eungjun Lee, Gibaek Lee*, Yongsug Tak* Department of Chemical Engineering, Inha University	B P2.18
14:00	Uniformly Decorated Graphene tube @ Graphene microsphere Hybrid for high rate supercapacitors Young Hwan Kim, Kwang Bum Kim* Department of Materials Science and Engineering, Yonsei University	B P2.6	14:00	Optical gain and radiative current density in 1.55 μm lattice-matched p-GaAs/-GaInAsB/n-GaAs multiple quantum well lasers I. Guizani, W.Q. Jemmal, M.M. Habbchi, A. Rebey University of Monastir, Faculty of Sciences, Unité de Recherche sur les Hétéro-Epitaix et Applications, 5019 Monastir, Tunisia	B P2.19
14:00	Core/shell structured Li₄Ti₅O₁₂/TiO₂ composite as anode materials for high performance of lithium ion battery Jun Hui Jeong, Byung-Hoon Park, Geon-Woo Lee, and Kwang-Bum Kim* Department of Material Science and Engineering, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Republic of Korea	B P2.7	14:00	Microstructure of the oxide-film due to thermal oxidation of TbFe₂ Krisna Marwani (1), J. Arout Chelvane (2), Emilia Pardo (1) (1) Department of Materials Science and Engineering, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar 382355, Gujarat, India, (2) Defence Metallurgical Research Laboratory, Kanchanbagh, Hyderabad 500056, India	B P2.20
14:00	SiO_x coated Li₄Ti₅O₁₂ composite for lithium ion battery with ultra-long cycle performance Jun Hui Jeong, Byung-Hoon Park, Geon-Woo Lee, and Kwang-Bum Kim* Department of Material Science and Engineering, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Republic of Korea	B P2.9	14:00	Kinetic and Comparative Study of the Isomerization Reaction of Substituted Icosadecane by DFT (TD-B3LYP) and Semi-empirical (AM1+PM6) Methods Z. SKANDERI 1, F. MECHACHITI 1, A. DJEBALI 1*, ILHEM, R. KRIBA 2 1 Laboratory of chemistry and environmental chemistry L.C.C.E - University of Batna 1- Algeria 2 Faculty of Sciences- Department of Physics - University of Batna 2- 05000- Algeria	B P2.23
14:00	Effects of nanoporeformation underneath SnO₂ in SnO₂/nanoporeformed graphene (NPQ) microball on lithium-ion storage performance Yeon Jun Choi, Myung Seong Kim, Jun Hui Jeong, Young Hwan Kim, and Kwang-Bum Kim Department of Material Science and Engineering, Yonsei University, 134 Shinchon-dong, Seodaemun-gu, Seoul, 120-749, South Korea	B P2.10	14:00	Synthesis and Characterization of Nickel Titanate as High Performance Anode for Rechargeable Lithium Ion Batteries Anita Majumder, Subhasan Basu, Rajkumar Materials Science Centre, Indian Institute of Technology, Kharagpur-721 302, India	B P2.24
14:00	Synthesis of SnO₂/nanoporeformed graphene (NPG) microball for high lithium-ion storage performance Yeon Jun Choi, Myung Seong Kim, Jun Hui Jeong, Young Hwan Kim, and Kwang-Bum Kim Department of Material Science and Engineering, Yonsei University, 134 Shinchon-dong, Seodaemun-gu, Seoul, 120-749, South Korea	B P2.11	14:00	Modeling of temperature profiles in the structure of a-Si-Sn-a-Si under the influence of different types of laser irradiation O.O. Havryluk, O.Yu. Semchuk O.Chulko Institute of Surface Chemistry NAS of Ukraine.	B P2.25
14:00	Mechanical alloying and the electrochemical properties of CaNi₅-based alloy 1 Youssef Dabaki, 1, 2 Mohamed Tilha, 1 ChokirKhalid, 3 NouredineFenneche, 4 Omar Elkedim, 1 LilianLamoum 1 University of Tunis, Laboratory of Mechanics, Materials and Processes, Group of Metal Hydrides, ENSIT, Tunisia 2 Department of Physics, University Faculty, Umm-Alqura University, Al-Qunudah, Saudi Arabia, 3 FEMTO-ST, CNRS-UTBM, Site Saverans, 90010 Belfort Cedex, France, 4 IRTES-LEMI-SPFR-FCIAB, Site de Sevenans, 90010 Belfort Cedex, France. * E-mail: dabakiyoussef@gmail.com	B P2.12	14:00	First principles calculations of the optical properties and polar (001) surfaces of Bi₂Se₃ R. I. Ego and A. I. Popov Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., Riga LV1063, Latvia, e-mail: regitis@gmail.com	B P2.26
14:00			14:00	Effect of N and Bi resonant states on the band structure and absorption coefficient of GaAs_{1-x}YnByGaAs strained quantum well N. Ajnef, W. Q. Jemmal*, M. M. Habbchi, A. Rebey University of Monastir, Faculty of sciences Monastir, Unité de Recherche sur les Hétéro-Epitaix et Applications / Corresponding author : *whedjemmal@gmail.com	B P2.27
			14:00	Self-powered system based on triboelectric wind energy harvesting Aravind RAVICHANDRAN, Marc FAMILUZ, Sylvain BLAYAC Aravind RAVICHANDRAN; Ph.D. student, Marc FAMILUZ; Asst. Professor, Sylvain BLAYAC; Thesis director	B P2.28

Ab initio design of BiCuO₅ derivatives as semiconductors for photochemical water splitting
 Anton Curutchet (1), Tangui Le Bahers (1), Amal BaQais (2,3), Ahmed Ziani (2), Hassan Ali Ahsane (2), Shikha Lardhi (2), Luigi Cavallo (2), Moussab Harb (2), Kazuhiro Takanebe (2), Philippe Sautet (4,5)
 (1) Univ Lyon, ENS de Lyon, CNRS, Université Claude Bernard Lyon 1, Laboratoire de Chimie UMR 5182, F-69342 Lyon, France (2) KAUST Catalysis Center (KCC) and Physical Sciences and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), P.O. Box 2460, 24550-2166, Thuwal, Saudi Arabia (3) Department of Chemistry, College of Sciences, Princess Nourah bint Abdulrahman University (PNU), Riyadh 11671, Saudi Arabia (4) Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, California 90095, United States (5) Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095, United States

Water Oxidation Chemistry of Oxynitrides and Oxides: Comparing NaTaO₃ and SrTiO₂N
 Hassan Ouhdi, Ulrich Aschauer
 Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland

Insights into Metal-CdS Interfaces (Metal= Ni, Pd, Pt, Au): Ab Initio Modelling of Clustered and Epitaxial Metal Depositions
 S.S. Gupta and M. A. van Huis
 Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University, Princetonplein 5, 3584 CC Utrecht, The Netherlands

Structural and electronic properties of Sr₂TaO₃N bulk and surfaces by density functional theory
 Maria Bouri, Ulrich Aschauer
 Department of Chemistry and Biochemistry, University of Bern, Switzerland

Effect of anion order and spontaneous polarisation on bandgaps in epitaxially strained oxynitrides
 Nathalie Vondt, Ulrich Aschauer
 Department of Chemistry and Biochemistry, University of Bern, Switzerland, Department of Chemistry and Biochemistry, University of Bern, Switzerland

Accelerated discovery of one-pot synthesizable heterojunctioned photocatalysts using machine learning
 Heoncheol Cho, Hyeonmin Khan, Sanghyun Han, Sehyun Chae
 1) Virtual Lab Inc., 2) Korea Institute of Science and Technology
 Coffee Break

New Methods and Resources for Materials Screening : S. Curtarolo

High Throughput Experimental Materials Database for Optoelectronic Energy Conversion
 Andriy Zakutayev, Nick Wunder, Marcus Schwaning, John D. Perkins, Robert White, Kristin Munch, William Tumas, Caleb Phillips
 National Renewable Energy Laboratory, Golden CO, USA

Novel theoretical crystal structure data in the ICSD database connecting theoretical and experimental material science
 D. Zagorac, J. Zagorac, H. Mueller, S. Rehme
 D. Zagorac, J. Zagorac, Institute of Nuclear Sciences Vinca, Materials Science Laboratory, Belgrade University of Technology and Architecture, Analysis, processing and characterization of materials for use in extreme conditions, "CEXTREME LAB" Laboratory for Theoretical Investigation of Materials (I-TIM), Belgrade, Serbia, H. Mueller, S. Rehme, FIZ Karlsruhe – Leibniz Institute for Information Infrastructure, Karlsruhe, Germany

Modeling Realistic TiO₂ Nanoparticles and Their Interaction with Water
 D. Selli, I. G. Fazio, I. G. Seifert, C. Di Valentin
 1) Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Milano, Italy 2) Technische Universität Dresden, Institut für Theoretische Chemie, D-01062 Dresden, Germany

Dynamics of highly excited electrons in semiconductors: theory and experiments.
 J. Sjakste
 Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS UMR 7642, CEA-DRF-IRAMIS, Paris-Saclay University, 91128 Palaiseau, France.