

# Mid-term Review

## Coordinator's Report

April 18, 2017 | Constantia Alexandrou |



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant Agreement No. 642069

- Introduction
- Management & Coordination
- Recruitment
- Training
- Research Work Packages
- Dissemination & Outreach
- Outlook
- References

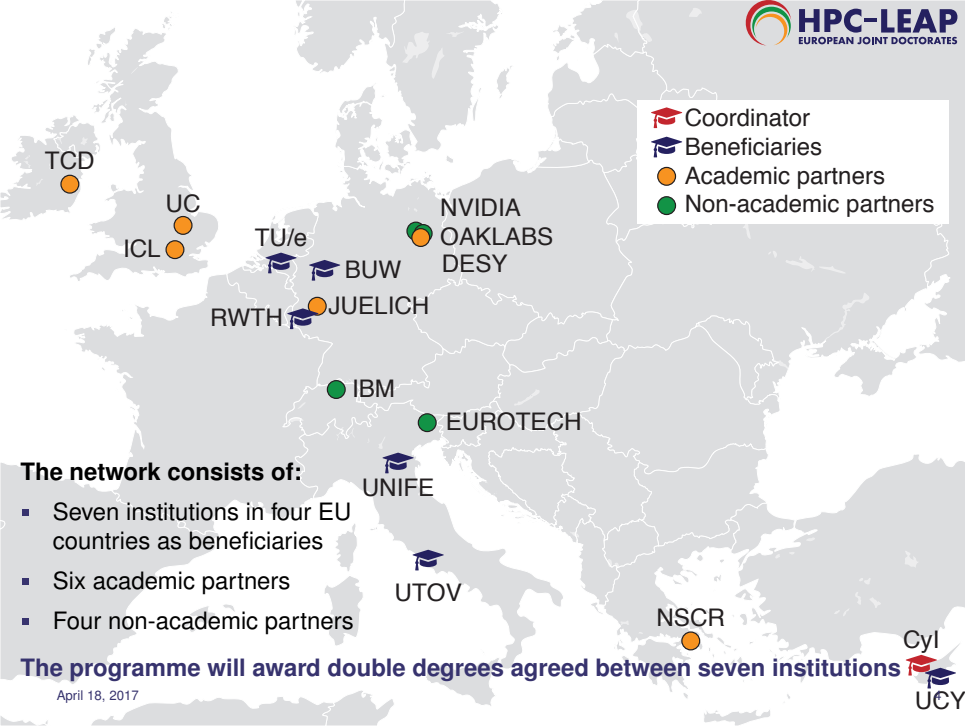
HPC-LEAP implements an interdisciplinary program for educating the next generation of scientists to use high performance computing in scientific inquiry.

The research areas are:

- Cross-disciplinary
  - HPC Architectures and Technologies
  - Mathematical Modelling and Algorithms
- Applications
  - Turbulent flows
  - Computational biology
  - Lattice Quantum Chromodynamics (QCD)

The research projects are designed to:

- Enhance collaborations and interactions across disciplines by engaging leading experts in HPC technologies, Applied Mathematics and Domain specific applications
- Integrate non-academic partners to prepare students for both academia and industry
- Develop HPC methodologies and algorithms for efficient usage of current and future computers → contribute towards Europe's competitiveness in HPC technologies



### The network consists of:

- Seven institutions in four EU countries as beneficiaries
- Six academic partners
- Four non-academic partners

**The programme will award double degrees agreed between seven institutions**

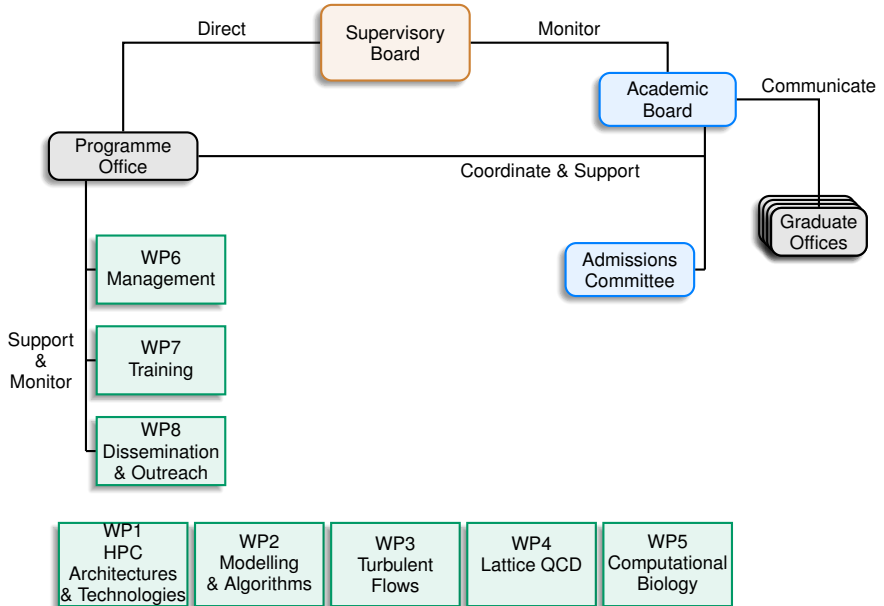
April 18, 2017

Formulation of dual-degree agreements:

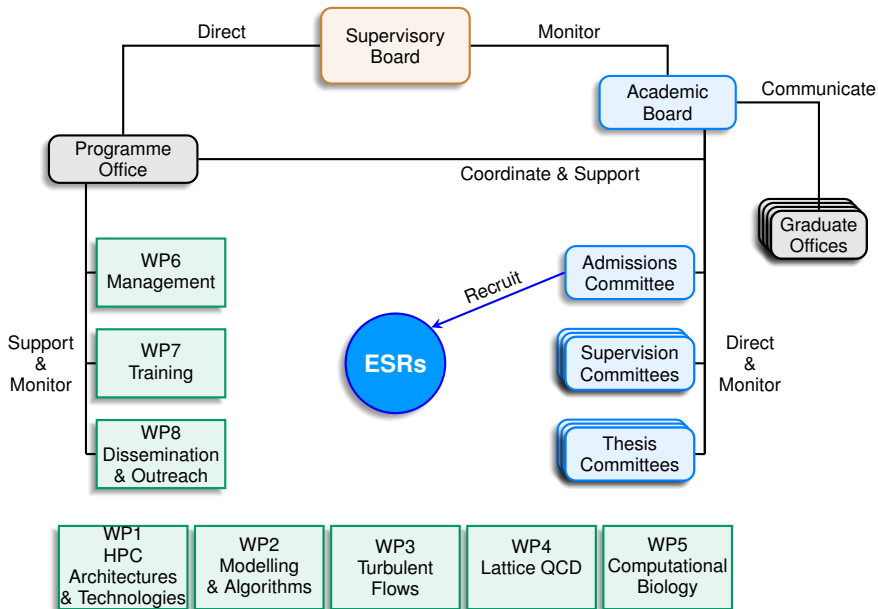
- General framework expendable beyond the duration of the project
- Flexible enough to take into account the requirements of both degree-awarding institutions
- Receiving strong administrative support from the seven degree-awarding institutions
- Seven dual-degree agreements across four EU countries (Cyprus, Germany, Italy and Holland):
  - Cyprus Institute and Wuppertal University
  - Cyprus Institute and Rome Tor Vergata
  - Cyprus Institute and Aachen University
  - University of Cyprus and Wuppertal University
  - Rome Tor Vergata and Aachen University
  - Rome Tor Vergata and TU Eindhoven
  - Ferrara University and Wuppertal University

## Part II: Management & Coordination

# Management structure

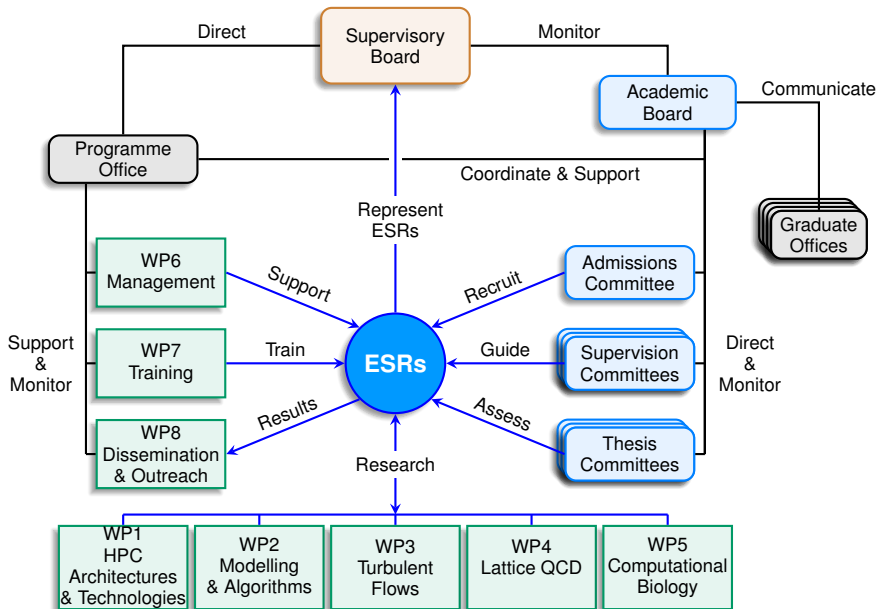


# Management structure





# Management structure



- The content and format of the workshops were determined by a committee led by the WP leader, the Project Coordinator and the scientists-in-charge of each workshop, which met in October 2014.
- The **Academic Board** met six times between December 2014 and April 2015 to
  - monitor the recruitment process
  - prepare the joint degree agreements
  - discuss the organisation of the workshops
- The **Supervisory Board** held five meetings throughout the reporting period to review and monitor all aspects concerning the implementation of the action, e.g.
  - budget matters
  - reporting
  - dissemination & outreach
  - event/workshop planning
  - scientific progress



Program for European Joint Doctorates  
High Performance Computing in Life sciences, Engineering and Physics

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## Thematic workshop on Lattice QCD at the physical pion mass: results, challenges and modern techniques

The workshop on Lattice QCD is part of the series of thematic workshops offered by the HPC-LEAP project. The workshop includes introductory lectures on scale setting and renormalization and will also cover topics on recent results using gauge configurations at or close to the physical pion mass, algorithmic developments (multigrid and multi-level techniques), as well as new developments such as the direct computation of PDFs. Insights into the challenges of these state-of-the-art lattice QCD simulations will be provided by some of the key researchers working in the area, who will share their results and experience on physical pion mass simulations.

Limited spaces are available for students & researchers that are not affiliated with the HPC-LEAP programme.

**Venue:** Stiftung Deutsches Elektronen Synchrotron (DESY), Zeuthen, Germany

**Dates:** 10 to 13 April 2017

To register and for further details visit the [website](#) of the workshop.

Registration for the workshop will remain open until **4 April 2017**.

## HPC-LEAP Students at the Researchers' Night 2016

### News

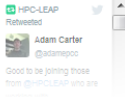
Thematic workshop on Lattice QCD at the physical pion mass: results, challenges and modern techniques

Fellowship position in Lattice QCD and HPC architectures

HPC-LEAP Students at the Researchers' Night 2016

### HPC-LEAP on Twitter

#### Tweets by @HPCLEAP



**[www.hpc-leap.eu](http://www.hpc-leap.eu)**

Website hosts information about the projects, the training and dissemination events, highlights and success stories

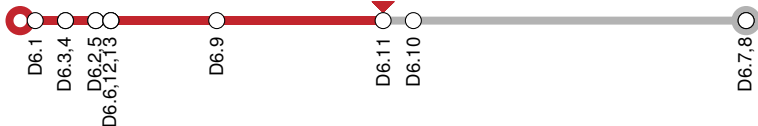
# Progress in WP6

## Management & Coordination - Deliverables

1 Apr 2015

31 Mar 2017

31 Mar 2019



### Deliverables

- D6.1 Project website (30 Apr 2015 - delivered by Oct 2014)
- D6.3 Recruitment completion (30 Jun 2015)
- D6.4 EJD Agreement (30 Jun 2015)
- D6.2 Kick-off meeting and SB meeting at Cyl (31 Aug 2015)
- D6.5 Declaration of Conformity (31 Aug 2015)
- D6.6 Career Development Plan (30 Sep 2015)
- D6.12 Supervisory board (30 Sep 2015)
- D6.13 ETHICS (30 Sep 2015)
- D6.9 Progress report (30 Apr 2016)
- D6.11 Draft period report (31 Mar 2017)

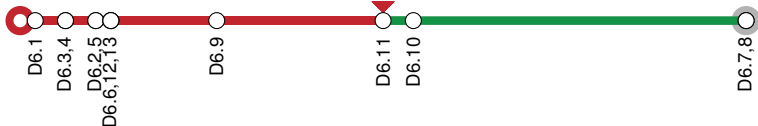
# Progress in WP6

## Management & Coordination - Deliverables

1 Apr 2015

31 Mar 2017

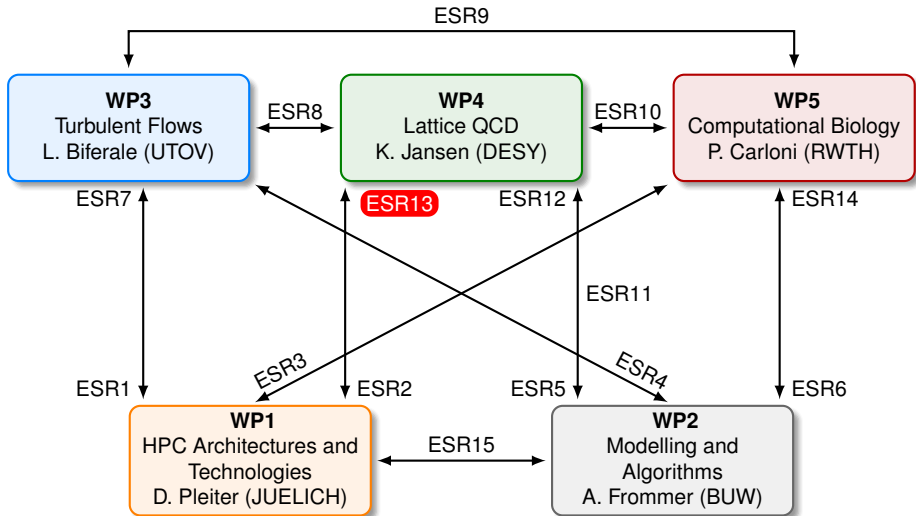
31 Mar 2019



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- D6.9 Progress report (30 Apr 2016)
- D6.11 Draft period report (31 Mar 2017)
- D6.10 Mid-term Report (31 May 2017)
- D6.7 Report on Ph.D. awards (31 Mar 2019)
- D6.8 Final project report (31 Mar 2019)

## Part III: Recruitment



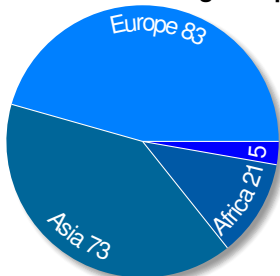
**Project starting date:** 1st April 2015

**Recruitment period:** November 2014 – April 2015

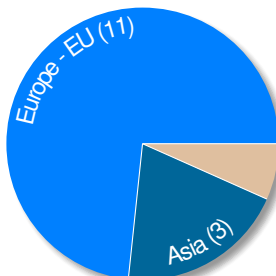
**Advertisement through:**

- EURAXESS portal
- Poster sent to institutions world-wide
- Science jobs websites
- HPC portals
- Supercomputing centres
- Personal contacts

**Considered 182 eligible applicants**



Applications per continent



Recruited Fellows



## Fifteen Marie Skłodowska-Curie Fellowships

Admission committees comprising of experts in each field

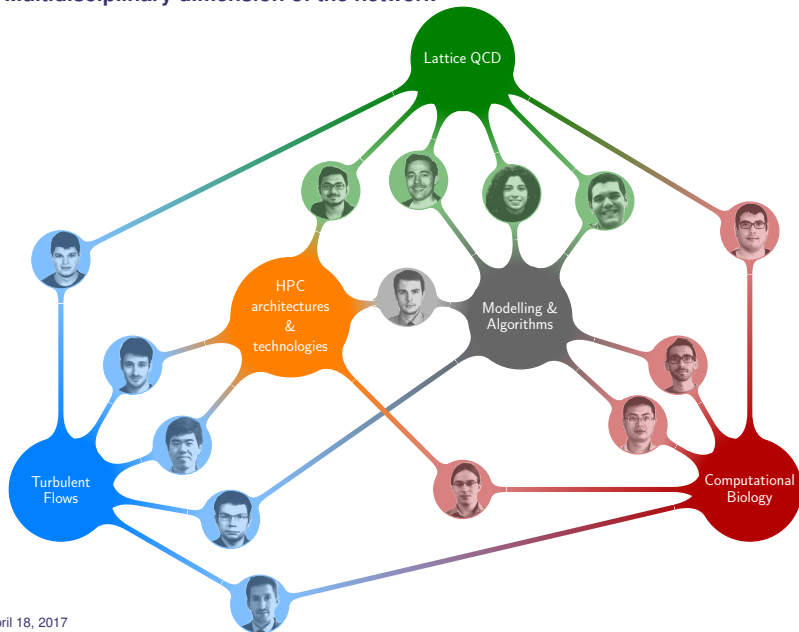
<b>Scientific Domain</b>	<b>ESR. No</b>	<b>SC members</b>
Computational Biology	6, 10, 14	P. Carloni, G. Christophides, G. Koutsou, A. Frommer K. Jansen, J. Kallarackal, K. Iatrou
Lattice QCD	11, 12, 13	H. Panagopoulos, F. Knechtli, C. Alexandrou, K. Jansen, M. Peardon, M. Wingate
Turbulent and Complex Flows	7, 8, 9	L. Biferale, F. Toschi, M. Sbragaglia, G. Fabio, K. Jansen, C. Alexandrou, M. Ehrhardt, P. Carloni, D. Pleiter, F. Knechtli
HPC Architectures and Technologies	1, 2, 3	R. Tripiccione, F. Knechtli, D. Pleiter, M. Ehrhardt G. Koutsou, A. Curioni, P. Carloni, G. Christophides, A. Curioni
Modeling and Algorithms	4, 5, 15	L. Biferale, M. Sbragaglia, F. Toschi, A. Frommer C. Alexandrou, F. Knechtli, A. Formmer, G. Fabio, D. Pleiter, S. Kraemer

Selection criteria needed to satisfy the academic admission criteria of two institutions:

- Academic excellence in undergraduate and master degrees
- Recommendation letters
- Research interests
- Interviews

# Synergies within HPC-LEAP

Multidisciplinary dimension of the network



## Part IV: Training

## Training organised by HPC-LEAP

- Four core workshops compulsory for all fellows
- One thematic workshop to be selected from the three domain specific areas

## Accreditation

- Each core workshop accredited with 5 ECTS units
- Each thematic workshop accredited with 3 ECTS, complemented with additional material at the nodes to give 7 ECTS units in addition
- These workshops satisfy most of the taught course requirements of the degree awarding institutions

## Organisation of workshops

- Content and format determined by a committee led by the WP7 leader (M. Peardon), with the participation of the Project Coordinator and the scientist(s)-in-charge of the node where the event was organized
- Designed to equip students with the necessary background for their HPC-driven research projects with hands-on exercises
- Core workshops focused on cross-disciplinary training providing interaction among the ESRs
- Open to students/researchers outside the network
- Quality assurance through feedback collected from students

# Core workshops

(ESRs attended all core workshops)

- 1 CoS-1a: School on numerical analysis and algorithms towards exascale (5 ECTS)**  
Venue: Wuppertal  
Dates: 23rd September - 13th October 2015  
Scientists-in-charge: Andreas Frommer and Francesco Knechtli
- 2 CoS-2a: School on HPC architectures and large-scale numerical computation (5 ECTS)**  
Venue: Jülich  
Dates: 11th - 29th Jan 2016  
Scientist-in-charge: Dirk Pleiter
- 3 CoS-1b: School on numerical analysis and algorithms at the exascale: Classical N-body methods for complex systems on massively parallel architectures (5 ECTS)**  
Venue: RWTH Aachen  
Dates: 5th - 22nd April 2016  
Scientist-in-charge: Paolo Carloni
- 4 Cos-2b: School on HPC architectures and numerical methods (5 ECTS)**  
Venue: Trinity College Dublin  
Dates: 13th June - 1st July 2016  
Scientist-in-charge: Mike Peardon

# Thematic workshops

(Each ESR attended one of the three workshops)

## **1 HPC Applications to Turbulence and Complex Flows (3 ECTS)**

Venue: Rome Tor Vergata

Dates: 10–14 October 2016

Scientist-in-charge: Luca Biferale

Attended by: Alessandro Gabbana, Felix Milan, Xiao Xue, Georgios Margazoglou, Guillaume Tauzin & Teodor Nikolov, which included 19 students outside the network.

## **2 Thematic workshop in Computational biology and applications in human health (3 ECTS)**

Venue: The Cyprus Institute

Dates: 24 October–4 November 2016

Scientist-in-charge: George Christophides

Attended by: Viacheslav Bolnykh, Wenping Lyu, Andrew Brockman & Thomas Tarenzi, including 5 students outside the network

## **3 Thematic workshop on Lattice QCD at the physical pion mass: results, challenges and modern techniques (3 ECTS)**

Venue: DESY, Zeuthen

Dates: 10–13 April 2017

Scientist-in-charge: Karl Jansen

Attended by: Srijit Paul, Simone Bacchio, Aurora Scapellato & Salvatore Calì and 30 researchers outside the network.

## Assessment for the core workshops

- Implementation of computer algorithms
- Small group or individual projects with short report and presentation

## Student Feedback

From the questionnaires administered at the end of core workshops

- Feedback has been generally positive on the organisation and content of the lecture material
- Students found the projects given as part of assessment interesting and at about the right level of difficulty.
- As expected, given the interdisciplinary nature of the project, the lecture schedule was rather intense for some students to digest all the material presented, especially on new subjects



Additional training opportunities were identified outside the network (14 training events/workshops/courses with some carrying ECTS accreditation). Examples include

- JMBC course on “Particle-based modelling techniques”, held at TUE, Oct 2015 (ESR7).
- “Lattice Practices 2015” at JULICH, Oct 2015 (ESR2, ESR5, ESR11, ESR12 and ESR13).
- Workshop on “Instantons and Extreme Events in Turbulence and Dynamical Systems” at IMPA, Brazil, Dec 2015 (ESR8).
- JMBC course “Turbulence”, University of Delft, May 2016 (ESR4, ESR7 and ESR8).
- CECAM workshop on “Structural and Functional Annotation of Bioinorganic Systems”, Scuola Normale Superiore, May 2016 (ESR3, ESR6, ESR10 and ESR14)
- CISM course “Multiscale modelling of flowing Soft Matter and Polymer Systems”, Jul 2016 (ESR4)
- Lattice2016, University of Southampton, Jul 2016 (ESR5).
- 9<sup>th</sup> International Workshop on Numerical Analysis and Lattice QFT, Edinburgh, Aug 2016 (ESR5).
- Course on “Advanced FORTRAN topics”, Sep 2016 (ESR3) .
- CECAM workshop “Atomistic Monte Carlo Simulations of Bio-molecular Systems”, JUELICH, Sep 2016 (ESR6)
- CECAM workshop “Water at interfaces: from proteins to devices”, University of Vienna, Dec 2016 (ESR6).
- Course on “Density Functional Theory and Electronic Structure”, RWTH, winter 2017 (ESR3).
- MARVEL School on variationally enhanced sampling, Università della Svizzera Italiana, Feb 2017, (ESR6).
- GPU Hackathon EuroHack 2017, at Jülich on GPU programming, Mar 2017 (ESR2, ESR3, ESR5, ESR9 and ESR15).


Sessions organised:

- During the last core workshop at Trinity College Dublin, the following sessions took place
  - Communication to the general public,
  - Creating a simple investment plan,
  - Introduction to patenting
- Tomorrow, 19 April 2017, four sessions will take place covering the following topics:
  - Communication in science
  - Negotiation and conflict management
  - Project and time management for Scientists
  - Experience working successfully in a company
- During the thematic workshops, domain-specific transferable skills were discussed (e.g. scientific writing, poster presentation).

Fellow	Host	Dates	Description of work
ESR2	JUELICH	16 Sep –18 Dec 2016	Implementations of Krylov solvers on NVIDIA Pascal GPUs using prototype machine JURON
ESR3	JUELICH	1 Oct 2016–1 Mar 2017	QM/MM implementation & development of testing projects
ESR4	BUW	1 Oct 2015 – 13 Oct 2015	Deflation-based methods for multilevel representations of the deflation subspace
ESR5	TCD	13 Jun–1 Jul 2016	Multigrid preconditioning for lattice QCD and hybrid MC with symplectic integrators
ESR8	JUELICH	11–29 Jan 2016	GPU programming, state-of-the-art techniques on performance analysis, modelling and optimisation for CPUs and GPUs
ESR8	DESY	15 Jul–15 Sep 2016	Benchmarking a hybrid MC code with respect to pseudospectral codes
ESR11	JUELICH	11–31 Jan 2016 11–30 Apr 2016	Optimisation techniques for lattice QCD
ESR11	DESY	2 Jul–5 Sep 2016	Theoretical and computational aspects of parton distribution functions
ESR12	TCD	1 Mar–2 Jul 2016	Noise dilution and distillation techniques for the evaluation of disconnected diagrams in hadron spectroscopy
ESR15	JUELICH NVIDIA	1 Feb–1 Sep 2017	Profiling and acceleration of asynchronous linear solvers on GPUs

## Supercomputing Training Portal

Home Practical HPC Development Improvement Visualisation **HPC-LEAP courses**



10 ▾

Title	Author	Hits
CoS-2b: School on HPC architectures and numerical methods	Written by Super User	<a href="#">Hits: 18</a>
CoS-1b: School on numerical analysis and algorithms at the exascale	Written by Super User	<a href="#">Hits: 9</a>
CoS-1: School on numerical analysis and algorithms towards exascale	Written by Super User	<a href="#">Hits: 31</a>

**[supercomputing.cyi.ac.cy](http://supercomputing.cyi.ac.cy)**

The portal hosts

- video recordings
- presentation slides

for three of the four core workshops. The recordings from the workshop at Jülich are in the process of being uploaded.

# Progress in WP7

## Training - Deliverables



### Deliverables

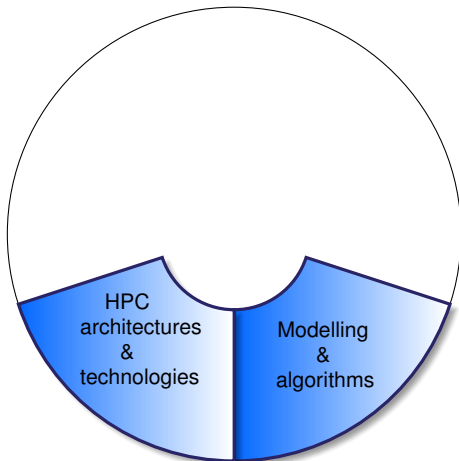
D7.1 Report on workshops (31 Mar 2017 - extension May 2017)



### Deliverables

- D7.1 Report on workshops (31 Mar 2017 - extension May 2017)
- D7.2 Report on shared courses (31 Mar 2018)
- D7.3 Project training portal (31 Mar 2019 )

## Part V: Research Work packages



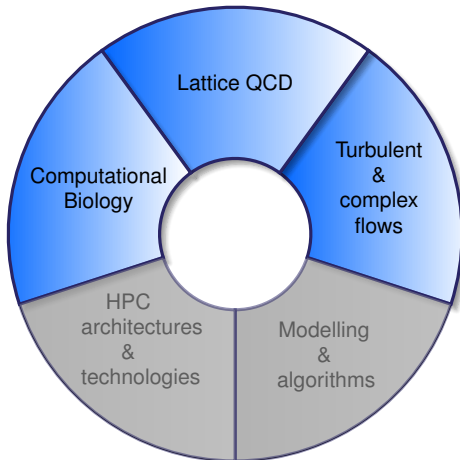
## WP1: HPC architectures & technologies

- Model the performance of algorithms on novel computer architectures
- Develop computational kernels for domain-specific applications

## WP 2: Modelling & Algorithms

- Improve existing simulation algorithms
- Develop new algorithms for current and future computer architectures
- Adjust algorithms to the domain of application e.g. multi-grid approaches





## WP3: Turbulence and Complex Flows

Understand and control turbulence and complex flows via numerical simulation, benefit from cross-fertilization

## WP4: Lattice QCD

Compute through large-scale simulations of lattice QCD observables relevant for beyond the standard model physics

## WP5: Computational Biology

Develop novel numerical methodologies to investigate biological molecules, including receptor/drug complexes

# Progress in WP1

## HPC architectures & technologies

- **ESR1** developed pilot applications using LBM on different HPC architectures and assessed their performance; he also developed and implemented a hybrid data structure to improve the utilisation of state-of-the-art heterogeneous architectures
- **ESR2** implemented successfully a multigrid CPU solver for lattice QCD on the NERSC systems; worked on porting the code on accelerators (Intel KNLs Xeon Phis, a major component of CORI); he also received training on how to implement algorithms on the latest GPUs of NVIDIA.
- **ESR3** developed a novel QM/MM interface which utilises a multiple-program multiple-data approach with a loose coupling between program components, a paradigm shift compared to previous implementations.
- **ESR15** explored existing HPC libraries, tools and languages for numerical linear algebra. The tool he developed for WP2 is hybrid parallel and works on a variety of architectures.



# Progress in WP1

## HPC architectures & technologies

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- **ESR3 Viacheslav Bolnykh**

- **ES** Developed a hybrid Quantum Mechanics/Molecular Mechanics interface
- **ES** Allows for HPC applications to QM phenomena in biological processes
- **ES** Collaboration with the Gromacs community to integrate this new interface into their implementation.



# Progress in WP1

## HPC architectures & technologies - Deliverables



### Deliverables

D1.1 Report on HPC architectures and technology trends (31 Mar 2016)

# Progress in WP1

## HPC architectures & technologies - Deliverables



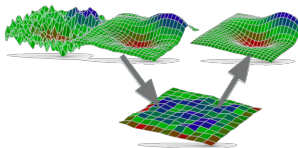
### Deliverables

- D1.1 Report on HPC architectures and technology trends (31 Mar 2016)
- D1.3 Report on potential exascale architectures (31 Jan 2018)
- D1.4 Further development of QM/MM codes for exascale (30 Sep 2018)
- D1.2 Report on LBM codes (31 Mar 2019 )

# Progress in WP2

## Modelling & Algorithms

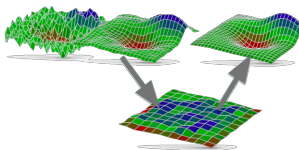
- **ESR2** developed an algorithm for lattice QCD based on multigrid preconditioning
- **ESR5** also developed a multigrid solver, extending a previous solver (DD- $\alpha$ MG) to the twisted mass fermion discretisation, observing a speedup between one and two orders of magnitude compared to previous methods. Received training on how to port features of his CPU multigrid code to GPUs.
- **ESR11** developed parallel algorithms for computing Parton Distribution Functions (PDFs) for lattice QCD to allow for the first direct calculation of PDFs at the physical point ensemble.
- **ESR12** implemented an algorithm which runs on multi-CPU architectures to capture the contributions of the disconnected diagrams to the estimation of meson masses, which were neglected in previous works.
- **ESR15** developed a novel approach for asynchronous iterative linear solvers to remedy some of the issues associated with poor convergence, by decoupling communication and iteration into separate threads. His project was accepted at Eurohack 2017 in order to receive training on how to port his library on GPUs.



# Progress in WP2

## Modelling & Algorithms

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- **ESR5** also developed a multigrid solver, extending a previous solver (DD- $\alpha$ MG) to the twisted mass fermion discretisation, observing a speedup between one and two orders of magnitude compared to previous methods. Received training on how to port features of his CPU multigrid code to GPUs.
- **ESR5 Simone Bacchio**
  - Supervised by A. Frommer to develop multigrid algorithms
  - Speedup improvements by two orders of magnitude to enable lattice QCD studies in hadron structure under the supervision of C. Alexandrou
  - Joint publication with UCY & BUW
  - Adopted in the ETMC software benefitting  $\sim 50$  scientists in Europe and the US leading to additional applications involving the fellow, see e.g. arXiv:1612.02061



# Progress in WP2

## Modelling & Algorithms - Deliverables



### Deliverables

- D2.1 Deflation algorithm (30 Sep 2016)
- D2.3 Domain decomposition algorithm (30 Sep 2016)



# Progress in WP2

## Modelling & Algorithms - Deliverables



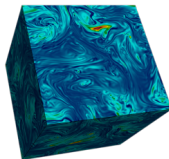
### Deliverables

- D2.1 Deflation algorithm (30 Sep 2016)
- D2.3 Domain decomposition algorithm (30 Sep 2016)
- D2.4 Multigrid algorithms (30 Sep 2017)
- D2.2 QCD algorithms (31 Mar 2018)
- D2.5 Multilevel methods (31 Mar 2019)

# Progress in WP3

## Turbulent flows

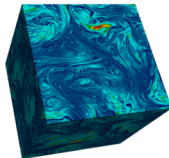
- **ESR1** introduced a new LBM for studying relativistic hydrodynamics, which bridges the gap between the previous theory on ultra-relativistic hydrodynamics all the way down to the non-relativistic regime.
- **ESR4** works on turbulent flows seeded with point-like and extended objects using LBM. He investigated droplet dynamics in synthetic time-dependent flows and is working towards replacing the external flow with a turbulent one.
- **ESR7** works on the formalism of LBMs with thermal fluctuations. He investigated ligament breakup in the presence of fluctuations; he is currently implementing a fluctuating LBM in HPC architectures to study the break-up of droplets by shear flows at the nanoscale.
- **ESR8** developed a serial and parallel version of a hybrid Monte Carlo code for random-force-driven prototypical turbulence models; he is also looking into extreme and very rare fluctuations, the so-called instantons, whose existence is connected with anomalous scaling and strong velocity fluctuations in small-scale turbulence.



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- **ESR4** works on turbulent flows seeded with point-like and extended objects using LBM. He investigated droplet dynamics in synthetic time-dependent flows and is working towards replacing the external flow with a turbulent one.

**ESR8 Georgios Margazoglou**

- Collaboration between lattice QCD and turbulent flows with UNIFE, DESY & UTOV
- Extended the range of applicability of Monte Carlo techniques to Stochastic Partial Differential Equations in general and to the case of Burgers' equations in particular.



# Progress in WP3

Turbulent and complex flows - Deliverables



**Deliverables**

# Progress in WP3

## Turbulent and complex flows - Deliverables



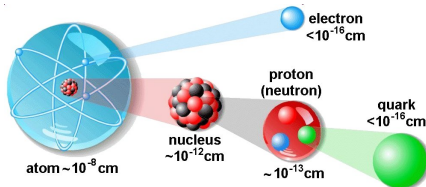
### Deliverables

- D3.3 Hybrid Monte-Carlo algorithms (31 Jul 2018)
- D3.4 Turbulence models in LBM (31 Jul 2018)
- D3.1 Algorithms for suspension hydrodynamics (31 Mar 2019)
- D3.2 Lattice Boltzmann Algorithms (31 Mar 2019 )

# Progress in WP4

## Lattice QCD

- **ESR2** developed a scattering phase shift analysis package, that allowed to obtain results at a higher accuracy, through an elaborate scheme which combines stochastic and sequential methods for calculating the contractions needed for the analysis.
- **ESR5** worked with the ETM collaboration to produce three ensembles at the physical point, where the pion mass is tuned to its physical values, which are of the largest lattice size produced by the ETM collaboration to date and will be utilised in the computation of disconnected diagrams.
- **ESR11** is working on computing parton distribution functions and proton form factors, by employing gauge configurations at the physical point ensemble with two light quarks, which is provided by the ETM collaboration.
- **ESR12** is investigating the effects of dynamical charm quarks on various observables. Due to their size, understanding their properties using simulations by extrapolating to zero lattice spacing is much more expensive computationally, as they require much finer lattices than the ones presently used with light quarks.



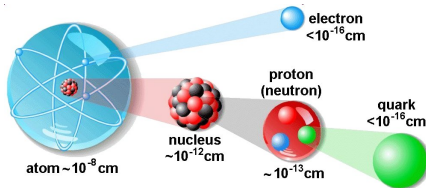
# Progress in WP4

## Lattice QCD

- **ESR2** developed a scattering phase shift analysis package, that allowed to obtain results at a higher accuracy, through an elaborate scheme which combines stochastic and sequential methods for calculating the contractions needed for the analysis.
- **ESR5** worked with the ETM collaboration to produce three ensembles at the physical point, where the pion mass is tuned to its physical values, which are of the largest lattice size produced by the ETM collaboration to date and will be utilised in the computation of disconnected diagrams.

### ESR2 Srijit Paul

- by ▪ Secondment to Jülich supervised by D. Pleiter
- qua ▪ Gained access to prototype GPU system JURON to learn performance modelling and optimize QUDA codes under the supervision of G. Koutsou
- ES ▪ Applied knowledge to study resonances in lattice QCD



# Progress in WP4

## Lattice QCD - Deliverables



### Deliverables





### Deliverables

- D4.3 Hadron spectrum and resonances (31 Mar 2018)
- D4.6 Renormalization constants (31 May 2018)
- D4.1 Nucleon structure and BSM physics (31 Jul 2018)
- D4.5 B to  $\pi$  and B to K decays (31 Jul 2018)
- D4.2 New approaches for disconnected diagrams (31 Mar 2019)
- D4.4 Time-like form factors (31 Mar 2019 )

# Progress in WP5

## Computational Biology

- **ESR3** utilises his massively parallel QM/MM interface for biomolecular research for projects related to biochemistry. The first of these study the tRNA cleavage catalysed by the Human Angiogenin, which can potentially yield insights into immunotoxin therapeutics development.
- **ESR6** worked on the HPC-based characterisation of biomolecules in mass spectrometry, by incorporating the previously neglected effects of proton dynamics and its impact on protein structural determinants and adopting a multistep simulation strategy on pharmacologically relevant peptides. He is also trying to gain insights into the high binding affinity of cisplatin (a potent anti-cancer drug) and DNA.
- **ESR10** undertook bioinformatics analyses for predicting protein–protein interactions (PPIs) between genes of *Anopheles gambiae* and *Plasmodium falciparum* and identified sets of manageable putative PPIs which are of relevance to medical and/or academic research.
- **ESR14** is working on a multiscale MD simulation method to improve the prediction of ligand binding poses and binding affinities specifically aimed for low-resolution protein models. He has also been working on the development of computational methods for mosquito GPCRs, which are targeted for anti-malaria interventions.



# Progress in WP5

## Computational Biology

- **ESR3** utilises his massively parallel QM/MM interface for biomolecular research for projects related to biochemistry. The first of these study the tRNA cleavage catalysed by the Human Angiogenin, which can potentially yield insights into immunotoxin therapeutics development.
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- ESR6 Wenping Lyu**

  - Undertook an HPC-based characterisation of biomolecules in mass-spectrometry
  - Accounted for previously neglected effects of proton dynamics
  - Results already published in a major journal of the field.
- **ES** (PF) ide aca
  - **ES** is working on a multiscale MD simulation method to improve the prediction of ligand binding poses and binding affinities specifically aimed for low-resolution protein models. He has also been working on the development of computational methods for mosquito GPCRs, which are targeted for anti-malaria interventions.



# Progress in WP5

## Computational Biology - Deliverables



### Deliverables

D5.5 Quantum Mechanics/Molecular Mechanics codes (30 Sep 2016)

# Progress in WP5

## Computational Biology - Deliverables



### Deliverables

- D5.5 Quantum Mechanics/Molecular Mechanics codes (30 Sep 2016)
- D5.3 Expression profiling tools (31 Mar 2018)
- D5.1 G-protein coupled receptors and SMLs (31 Jul 2018)
- D5.2 REL1 and other transcription factors (30 Sep 2018)
- D5.4 Coarse Grain/All Atoms code (31 Mar 2019 )

The ESRs have contributed to successful proposals for obtaining CPU time. Examples include:

- **Simone Bacchio (ESR5) and Aurora Scapellato (ESR11)**
  - “Nucleon observables as probes for physics beyond the standard model” (pr74yo) on the GCS Supercomputer SuperMUC at Leibniz Supercomputing Centre (80 million core-h).
  - nph116, **Titan - largest in US** at Oak Ridge Leadership Computing Facility (50 million core-h).
- **Salvatore Calì (ESR12)**
  - “Charm loops effects” on the GCS supercomputer (68 million core-h on JUQUEEN; 2 million core-h on JURECA; applied for 46 million core-h on JUQUEEN and 1 million core-h on JURECA to finish computations).
- **Georgios Margazoglou (ESR8)**
  - “BurgersHMC Instantons and Intermittency in Hydrodynamic Turbulence: A Lattice Monte Carlo Approach” on the **Marconi KNL - biggest in Italy** (Cineca, Italy) under the 13th PRACE call (18 million core-h).
- **Viacheslav Bolnykh (ESR3)**
  - Cy-Tera, project id: pro16b118s1 (105,000 core-h).
  - JURECA, project id: jias55 (450,000 core-h).
- **Wenping Lyu (ESR6)**
  - “Structural predictions of platinated DNA in complex with HMGB1A protein in quasi in vivo conditions”, ARA-HPC+VSR Project, **JUQUEEN-second biggest in Germany** (17 million core-h).
- **Thomas Tarenzi (ESR14)**
  - “Ligand binding to the OR7D4 odorant receptor studied by multiscale molecular simulations”, JARA-HPC, RWTH Compute Cluster (349,992 core-h).
  - “Ligand binding to bitter taste receptors studied by multiscale molecular dynamics simulations”, OCuLUS Cluster, Paderborn, Germany (864,000 core-h awarded).

## Part VI: Dissemination & Outreach

A detailed dissemination plan for the first two years of the project was prepared by WP8 leader M. Wingate

## Publications

- Published peer-reviewed articles: 6
- Conference proceedings: 6
- Submitted/in preparation: 10

## Open access

All the publications of the network are uploaded to the arXiv of the specific area and to the HPC-LEAP website

## Talks/posters

Besides the engagement of the ERSs in presentations during the thematic workshops, we had

- 8 ESRs have engaged in at least one dissemination activity
- 25 dissemination activities in total (10 conference talks, 12 posters and 3 seminar talks)

## Open source codes

- Contribution to the open source QUDA in collaboration with NVIDIA main developer based in the US
- Eight projects were made openly available on GitHub



- **A three-day kickoff meeting of HPC-LEAP** in Cyprus with the participation of all ESRs and scientists involved (14-16 September 2015).  
Included:
  - A Public event opened by the minister of Education and Culture of Cyprus with presentations by the leaders of all scientific work package and Jim Kallarackal, the CEO of OAKLABS on how to start a company
  - Organization of ESRs in outreach subgroups targeting different groups of people (undergraduates, high school students, general public, for addressing issues on gender equality) to investigate outreach opportunities



- **Established a social identity for HPC-LEAP** on facebook, twitter and linkedin
- **Fellows contributed blog posts** about their initial experiences into HPC-LEAP

- **European Researchers' Night**, e.g. in Cyprus involving four students



- **Open Days**, e.g. at UNIFE, 11-16 October 2016, presentation by Alessandro Gabbana.
- **Talks to undergraduates**, e.g. by Georgios Margazoglou during the DESY Summer Student Programme, August 2016
- **A concept for a documentary** “Women in HPC: to inspire high school students” by Fellow Andrew Brockman discussed with filmmaker and former sports journalist Mei Leng-yew.

# Progress in WP8

## Dissemination & Outreach - Deliverables



### Deliverables

- D8.1 Dissemination and outreach plan (31 Jul 2015)
- D8.2 Year-1 Dissemination report (31 Mar 2016)
- D8.3 Year-2 Dissemination report (31 Mar 2017)
- D8.8 Project dissemination material (31 Mar 2017 - extension until 31 Dec 2017)**

## Dissemination & Outreach - Deliverables



### Deliverables

- D8.1 Dissemination and outreach plan (31 Jul 2015)
- D8.2 Year-1 Dissemination report (31 Mar 2016)
- D8.3 Year-2 Dissemination report (31 Mar 2017)
- D8.8 Project dissemination material (31 Mar 2017 - extension until 31 Dec 2017)**
- D8.4 Year-3 Dissemination report (31 Mar 2018)
- D8.9 Report on conference (30 Nov 2018)
- D8.5 Final Dissemination report (31 Mar 2019)
- D8.6 ATLANTIS project HiPOP website (31 Mar 2019)
- D8.7 Scientific publications report (31 Mar 2019)

# Publications

## Peer-reviewed

- 1 Calore, E., Gabbana, A., Kraus, J., Schifano, S. F. & Tripiccione, R. (2016) Performance and portability of accelerated lattice Boltzmann applications with OpenACC. *Concurrency and Computation: Practice and Experience*, **28**, 34853502. arXiv: 1703.00186.
- 2 Calore, E., Gabbana, A., Kraus, J., Pellegrini, E., Schifano, S. & Tripiccione, R. (2016) Massively parallel lattice Boltzmann codes on large GPU clusters. *Parallel Computing*, **58**, 124. arXiv: 1703.00185.
- 3 Alexandrou, C., Bacchio, S., Finkenrath, J., Frommer, A., Kahl, K. & Rottmann, M. (2016) Adaptive aggregation-based domain decomposition multigrid for twisted mass fermions. *Physical Review D*, **94**, 114509. arXiv: 1610.02370.
- 4 Li, J., Lyu, W., Rossetti, G., Konijnenberg, A., Natalello, A., Ippoliti, E., Orozco, M., Sobott, F., Grandori, R. & Carloni, P. (2017) Proton dynamics in protein mass spectrometry. *The Journal of Physical Chemistry Letters*, **8**, 11051112. arXiv: 1702.07929.
- 5 Calore, E., Gabbana, A., Schifano, S. F. & Tripiccione, R. (2017) Evaluation of DVFS techniques on modern HPC processors and accelerators for energy-aware applications. *Concurrency and Computation: Practice and Experience*. Published Online 29 Mar 2017. arXiv: 1703.02788.
- 6 Calore, E., Gabbana, A., Schifano, S. F. & Tripiccione, R. (2017) Optimization of lattice Boltzmann simulations on heterogeneous computers. *The International Journal of High Performance Computing Applications*. In press March 2017. arXiv: 1703.04594.

# Publications

## Articles in conference proceedings

- 7** Leskovec, L., Alexandrou, C., Koutsou, G., Meinel, S., Negele, J. W., Paul, S., Petschlies, M., Pochinsky, A., Rendon, G. & Syritsyn, S. (2016) A study of the radiative transition  $\pi\pi \rightarrow \pi\gamma^*$  with lattice QCD. In: PoS (LATTICE2016), 159 (7 pages). arXiv: 1611.00282.
- 8** Liu, L., Bacchio, S., Dimopoulos, P., Finkenrath, J., Frezzotti, R., Helmes, C., Jost, C., Knippschild, B., Kostrzewa, B., Liu, H., Ottnad, K., Petschlies, M., Urbach, C. & Werner, M. (2016) Isospin-0  $\pi\pi$  scattering from twisted mass lattice QCD. In: PoS (LATTICE2016), 119 (7 pages). arXiv: 1701.08961.
- 9** Bacchio, S., Alexandrou, C., Finkenrath, J., Frommer, A., Kahl, K. & Rottmann, M. (2016) DDalphaAMG for twisted mass fermions. In: PoS (LATTICE2016), 259 (7 pages). arXiv: 1611.01034.
- 10** Korzec, T., Knechtli, F., Calì, S., Leder, B. & Moir, G. (2016) Impact of dynamical charm quarks. In: PoS (LATTICE2016), 126 (7 pages). arXiv: 1612.07634.
- 11** Alexandrou, C., Constantinou, M., Hadjiyiannakou, K., Kallidonis, C., Koutsou, G., Jansen, K., Wiese, C. & Vaquero Avils-Casco, A. (2016) Nucleon spin and quark content at the physical point. In: PoS (LATTICE2016), 153 (7 pages). arXiv: 1611.09163.
- 12** Alexandrou, C., Cichy, K., Constantinou, M., Hadjiyiannakou, K., Jansen, K., Steffens, F. & Wiese, C. (2016) Parton distributions from lattice QCD with momentum smearing. In: PoS (LATTICE2016), 151 (7 pages). arXiv: 1612.08728.

# Publications

## Submitted and in preparation

- 13** Gabbana, A., Mendoza, M., Succi, S. & Tripiccone, R. (2017) Kinetic approach to relativistic dissipation. *Physical Review Letters*. Submitted April 2017. arXiv: 1704.02523.
- 14** Gabbana, A., Mendoza, M., Succi, S. & Tripiccone, R. (2017) Towards a unified lattice kinetic scheme for relativistic hydrodynamics. *Physical Review E*. Submitted Dec. 2016. arXiv: 1703.04605.
- 15** Liu, L., Bacchio, S., Dimopoulos, P., Finkenrath, J., Frezzotti, R., Helmes, C., Jost, C., Knippschild, B., Kostrzewa, B., Liu, H., Ottnad, K., Petschlies, M., Urbach, C. & Werner, M. (2017) Isospin-0  $\pi\pi$  s-wave scattering length from twisted mass lattice QCD. *Physical Review D*. Under review (21 pages). arXiv: 1612.02061.
- 16** Lyu, W., Rossetti, G., Christophides, G., Natile, G., Arnesano, F. & Carloni, P. Effect of post-translational modifications of HMGB1 box-A on the interface of cisplatin-DNA adducts. In preparation.
- 17** Brockman, A., MacCallum, R. & Christophides, G. HPC DREME for unsupervised multi-species Cis regulatory element detection. In preparation.
- 18** Tarenzi, T., Calandrini, V., Potestio, R., Giorgetti, A. & Carloni, P. Multiscale simulation approach for accurate drug affinity predictions using low-resolution protein models. In preparation.

# Publications

Submitted and in preparation

- 19** Alexandrou, C., Cichy, K., Constantinou, M., Hadjiyiannakou, K., Jansen, K., Steffens, F. & Wiese, C. (2016) New lattice results for parton distributions. arXiv: 1610.03689.
- 20** Friedrich, J. and Margazoglou, G. & Biferale, L. and Grauer, R. Different routes for understanding the dissipation anomaly in turbulence. *Physical Review E*. In preparation.
- 21** Biferale, L., Jansen, K., Margazoglou, G., Mesterhazy, D., Rosenow, T. & Tripiccone, R. (2017) Hybrid Monte Carlo importance sampling for large fluctuations in nonequilibrium stochastic field theories. *Computer Physics Communications*. In preparation.
- 22** Gupta, A., Belardinelli, D., Sbragaglia, M., Xue, X. & Toschi, F. (2017) Effects of thermal fluctuations in geometry mediated droplet break-up: a Lattice Boltzmann Study. *Physical Review E*. In preparation.



HPC-LEAP is a very demanding interdisciplinary project covering topics from fundamental physics to biological systems and involving complex mathematical concepts and code development.

- An intensive training program for the ESRs with core skills that transcend the usual domain-specific training
- Higher than average mobility requirements for the fellows
- Close collaboration between the two supervisors and coordination with the scientist in-charge for the secondments
- Constant oversight of the program office for the satisfaction of the degree requirements of both degree-awarding institutions

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- The fellows have performed exceptionally well within the interdisciplinary environment of the project
- Despite the intense one-year long training program, significant research outcomes have been realized some of which are already published
- Research breakthroughs have been achieved that would not have been possible without the dual supervision
- Admission and supervision procedures have been streamlined by institutions across Europe → can lead to sustainable structures e.g. in seeking further common funding and recruitment of students

Examples:

- A new EJD with **joint** degrees amongst 3 three institutions currently under review
- A new EID currently under review