Exhibitor Forum Take Over!

May 22, 2023

WHPC
WOMEN IN HPC

Welcome!

Frank Herold
CEO, BeeGFS

Deb Goldfarb
Director of Product and Strategy for HPC & Batch, AWS

Cristin Merritt
CMO, Alces Flight

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Agenda - Part One

- **Welcome**
- **SPECIAL ANNOUNCEMENT**
- **WHPC Chapters + Affiliates** – *Cerlane Leong and Sadaf Alam*
- **In Support of Diversity + Inclusion** – *Frank Herold, BeeGFS*
- **Early Career Speakers!**
  - *Carla Santana, Universidade Federal do Rio Grande do Norte*
  - *Stefanie Reuter, University of Cambridge*
  - *Elisabeth Ortega, HPCNow!*
  - *Jenny Wong, University of Birmingham*

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Agenda - Part Two

- **In Support of Diversity + Inclusion** – *Deb Goldfarb, AWS*
- **Early Career Speakers!**
  - *Paula Esposito, La Laguna University*
  - *Aleksandra Kowalczuk, University of Warsaw*
  - *Ekaterina Zossimova, University of Exeter*
  - *Helena Vela Beltran, Barcelona Supercomputing Center*
- **Close!**

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Supporting Institutions - Career

Supporting Institutions - Volunteer

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Talk to us today about how you can fund our global initiatives!

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How to get involved!

Join Women in HPC for FREE!

- Select a Chapter/Affiliate for local events
- Let us know if you would like to get involved:
  - SC23 – Denver, USA
  - ISC 2024

womeninhpc.org

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Poster Reception

May 23, 2023

Foyer D-G

3:30 - 5:30 PM

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Grab your swag!

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Special Announcement

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Chapters and Affiliates

ISC2023

May 22nd, Hamburg

Women in High Performance Computing (WHPC)
Stewarded by EPCC at the University of Edinburgh, UK
The University of Edinburgh is a charitable body, registered in Scotland with registration number SC005336

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WHPC works with Chapters and Affiliates to support and promote the work of women in their organizations, develop crucial role models, and assist employers in the recruitment and retention of a diverse and inclusive HPC workforce.

Around 20 Chapters are active today worldwide

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7 Chapters are present in Europe, out of which 3 started in 2023:

-JuWinHPC at JSc in Juelich
contact : Ruth Schoebel and Claire Wyatt

-BSC in Barcelona
contact: Marta Garcia

-IDEAS4HPC in Switzerland
not-for-profit association
contact : see next slide

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Contact

Maria GIRONE, Director CERN OpenLab, Vice President

Cerlane LEONG, Senior Computer Scientist at ETHZ CSCS, Treasurer

Prof. Florina CIORBA, Head of HPC group of University of Basel, Secretary

Marie-Christine SAWLEY, HPC Advisor ICES Foundation Geneva, President

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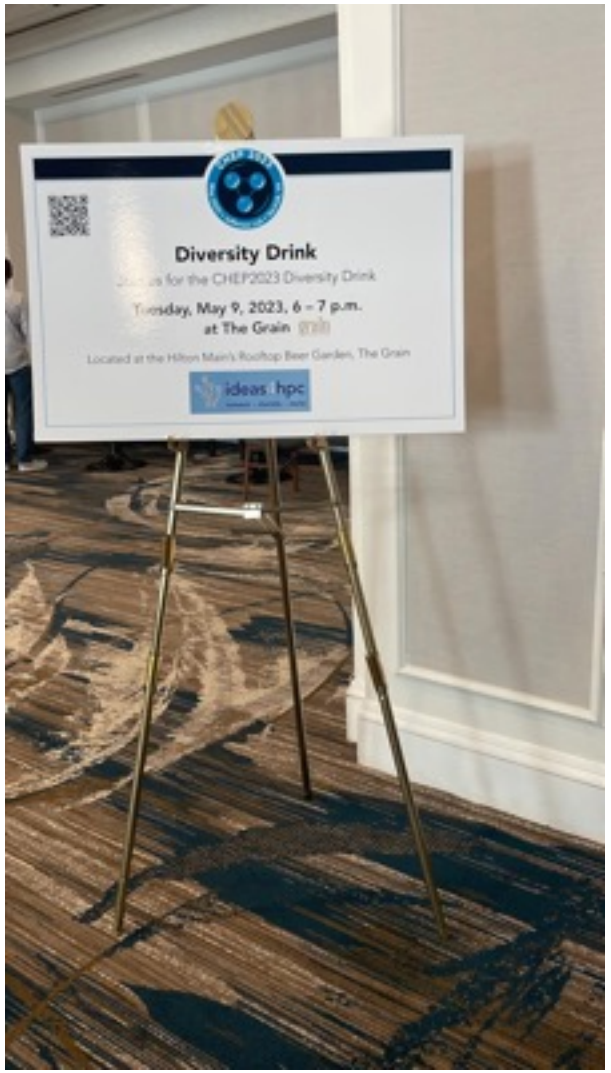
ACTIVITIES



https://www.jlab.org/conference/CHEP2023

ISC High Performance
The HPC Event.
WHPC

exhibitor forum take over
22 May 2023

PASC23
Davos Switzerland | 26-28 June 2023

Mini-Symposium:
Breaking the Silos to Enhance HPC Impact
27 June 2023, 16:00—18:00

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Women in HPC

Frank Herold

CEO, BeeGFS

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Early Career Speakers

Carla Santana
Universidade Federal do Rio Grande do Norte

Stefanie Reuter
University of Cambridge

Elisabeth Ortega
HPCNow!

Jenny Wong
University of Birmingham

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DeLIA: Dependability Library for Iterative Applications

Carla dos Santos Santana, Idalmis Milian Sardina,
Hervé Chauris, Claude Tadonki, Samuel Xavier de Souza

Summary

- Motivation
- DeLIA Features
- Case Study: 3D Full Waveform Inversion
- DeLIA Usability
- Next steps

Motivation

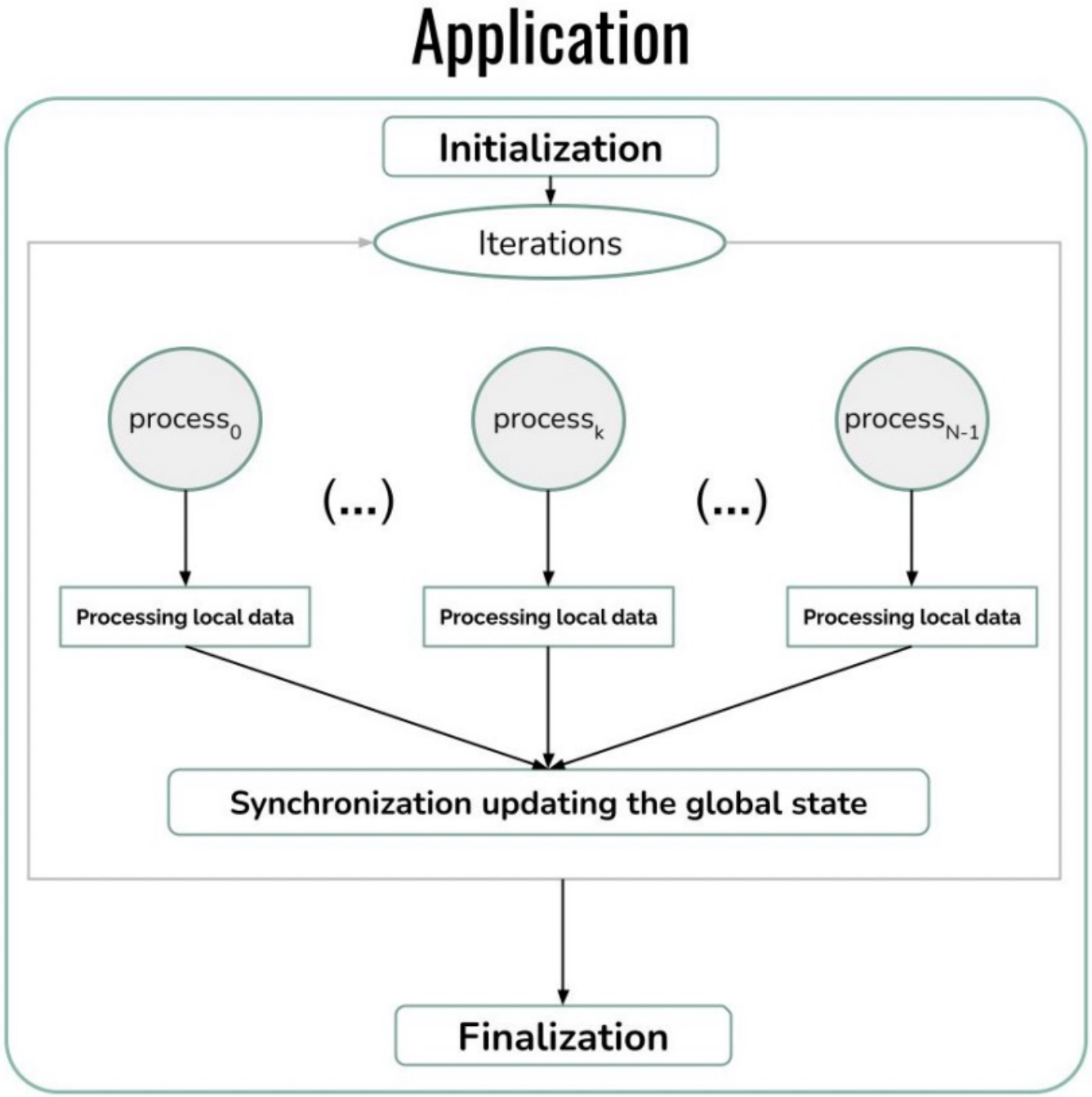
- One of the primary purposes of an HPC implementation is **scalability**.
- However, with more nodes, the probability of failure is higher.
- An execution of HPC application can be interrupted
  - Some failure in the HPC environment (e.g. network failures).
  - Preemptive circumstances (e.g. cloud instances preemptives).
- Therefore, dealing with faults is crucial for a scalable HPC application [4].

Motivation

Developing fault tolerance techniques that
do not cause significant overheads.

- HPC Applications
  - Many data
  - Many calculations
  - Spends a lot time to be complete
  - Fast

Application Behavior



DeLIA Features

Interruption Detection

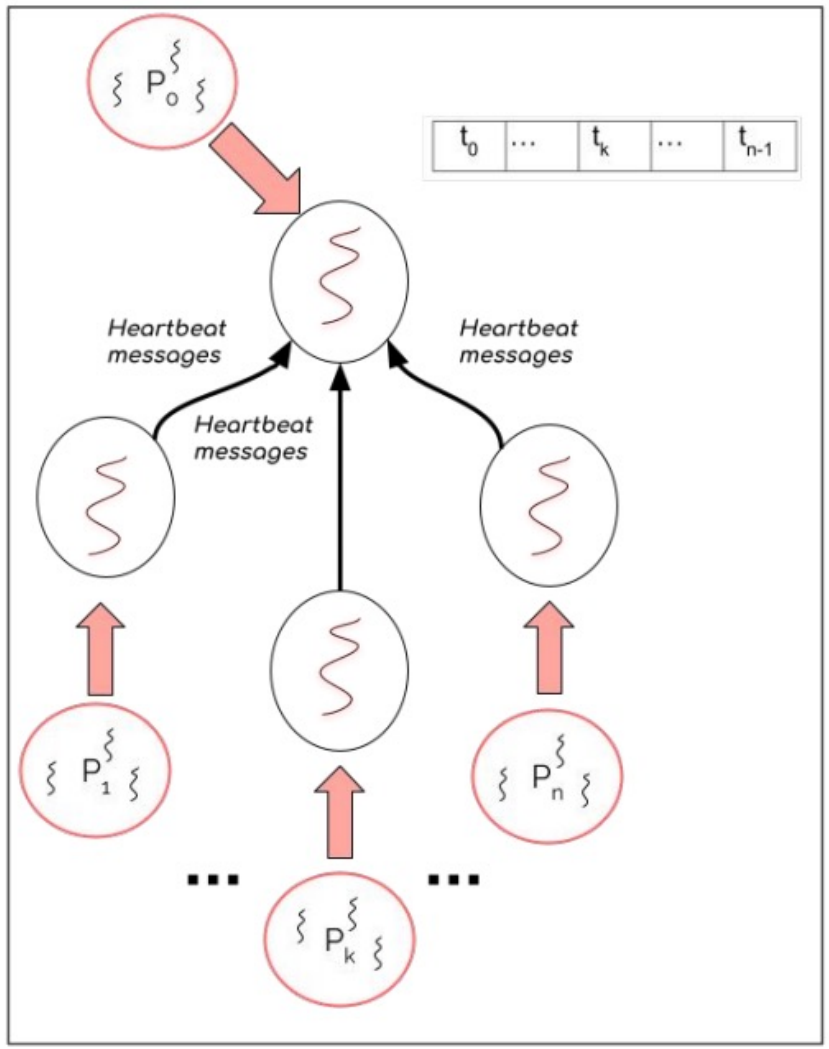
- Fault detection with the method of Heartbeat Monitoring
- Detection of termination signals.

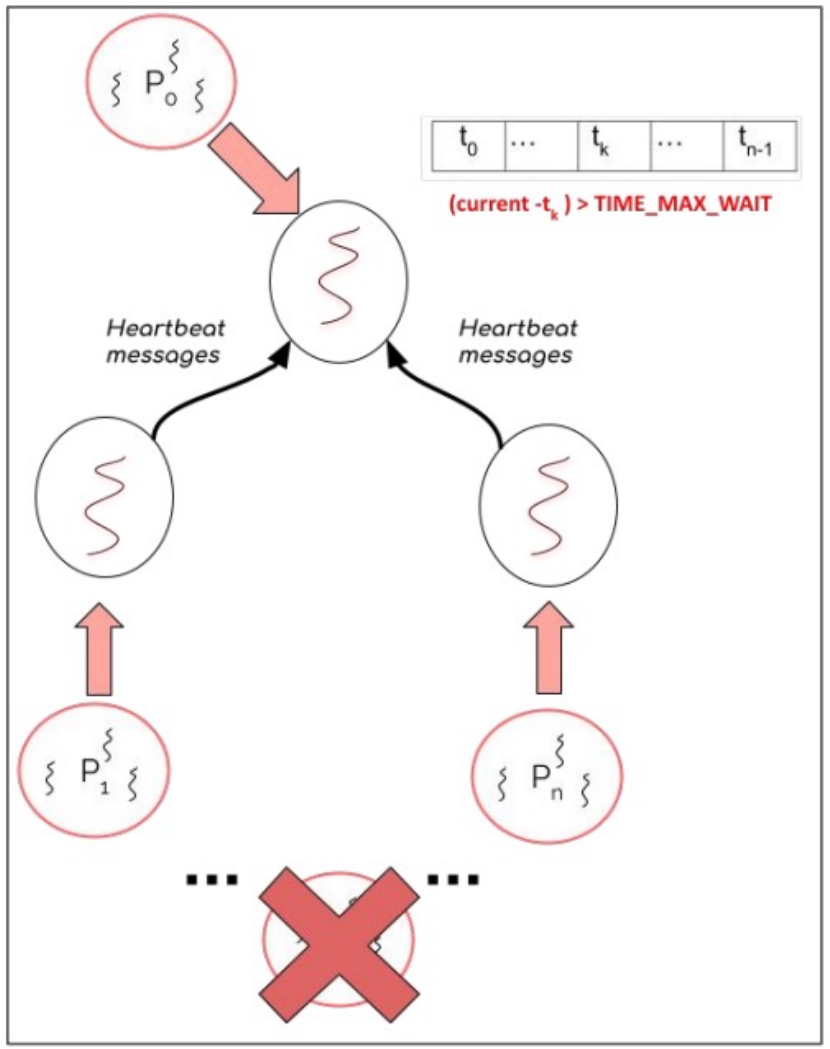
If **there is a possibility of interruption**,

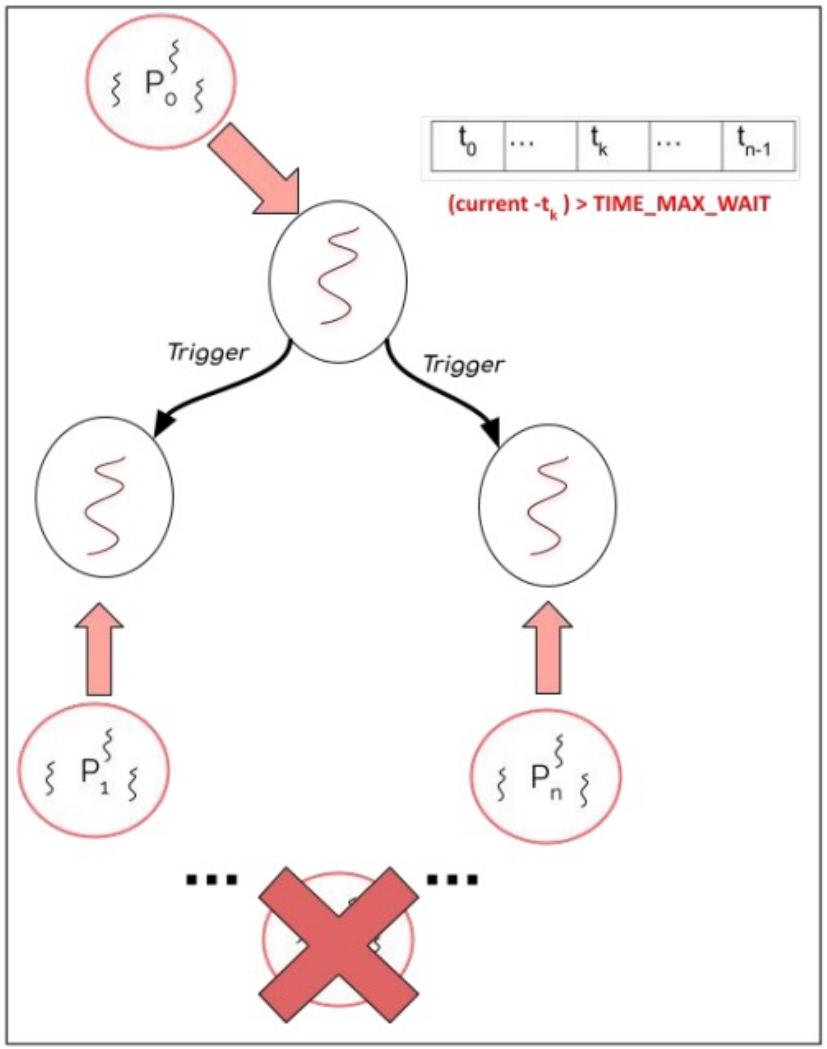
a trigger is sent to the nodes, and each one saves its local data

DeLIA Features

Heartbeat Monitoring







DeLIA Features

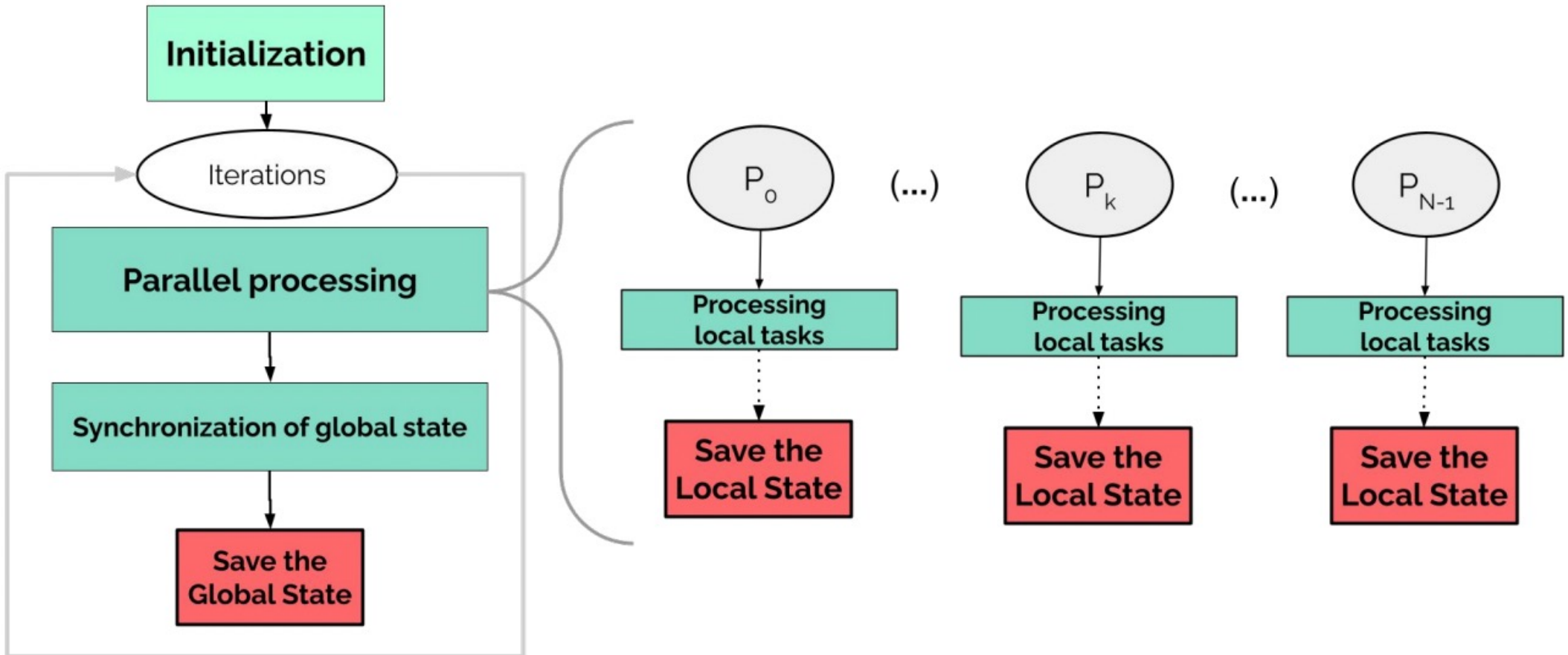
Detection of Termination Signals

- Interruption Signal are applied to advise a process that will probably terminate at some moment.
- Some supercomputers and cloud systems use them to notify a job that it will finish for some reason.
- In DeLIA:
  - When an termination signal is detected a trigger is send to the process.

DeLIA Features

Checkpointing and Rollback

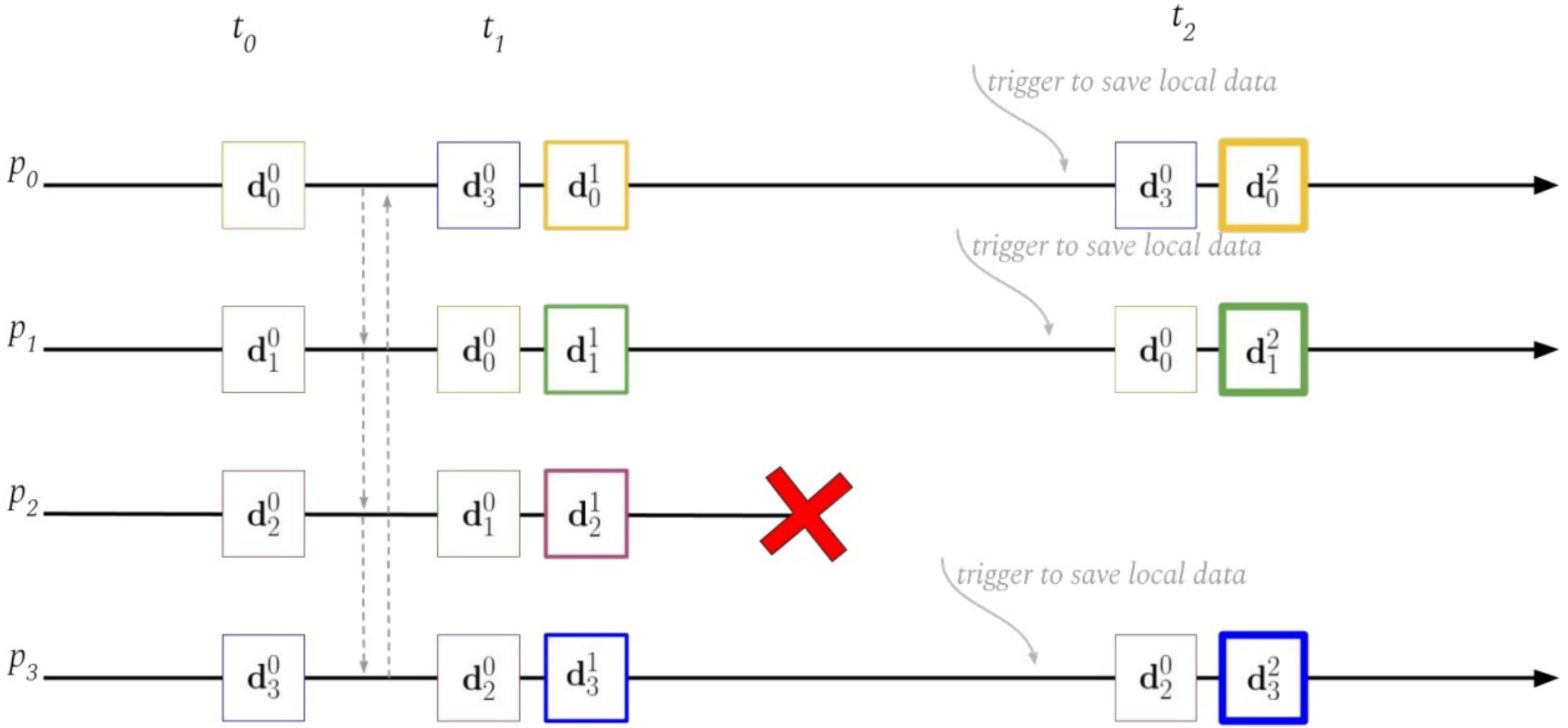
Checkpointing is the technique to save the data in a determined state. This can be used to resume the process later [5].



DeLIA Features

Replication

Replication of data is the most typical means to provide high availability and fault tolerance in distributed systems [2]



Case Study: 3D Full Waveform Inversion

Overview

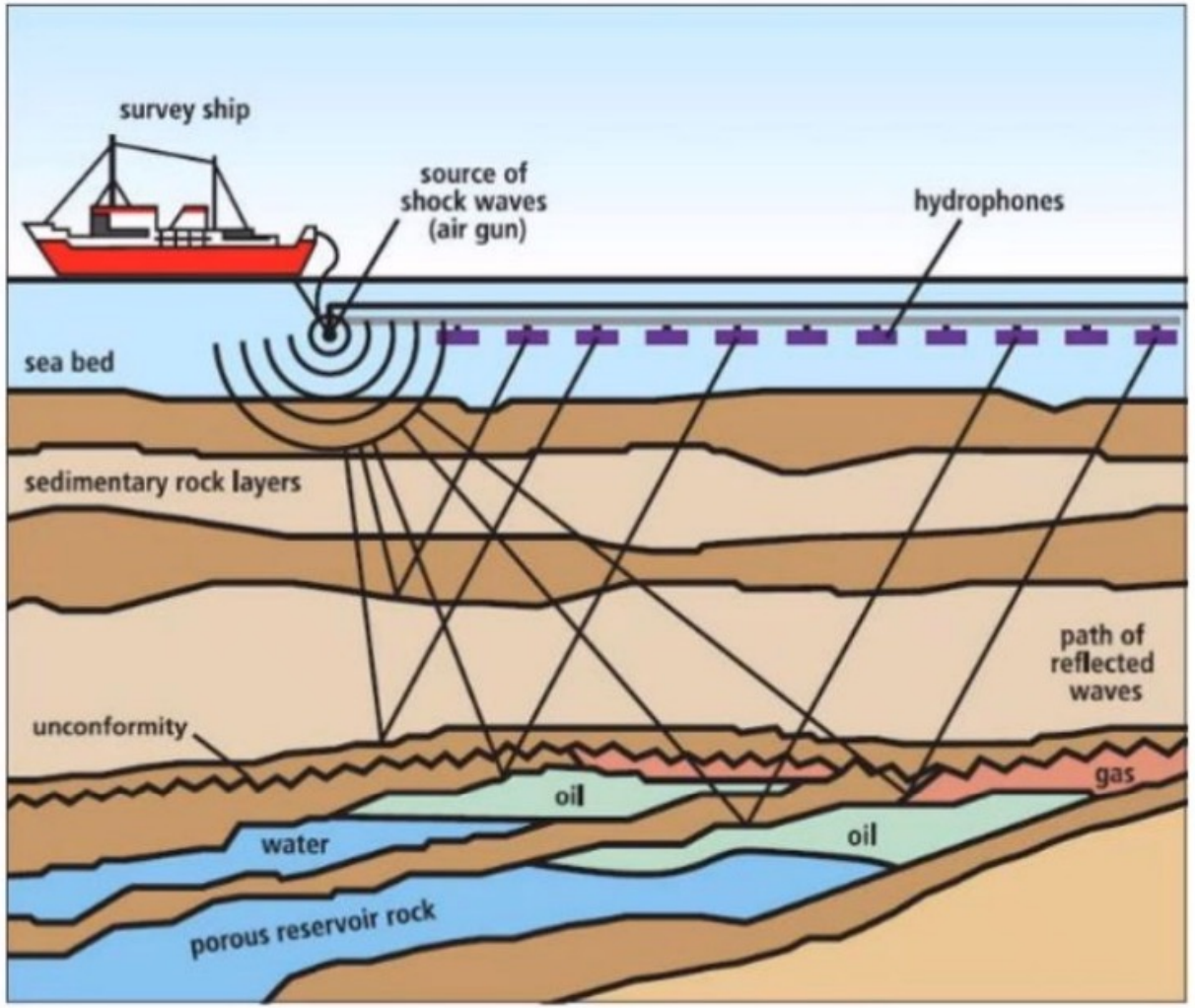


Figure from [3]

Case Study: 3D Full Waveform Inversion

Overview

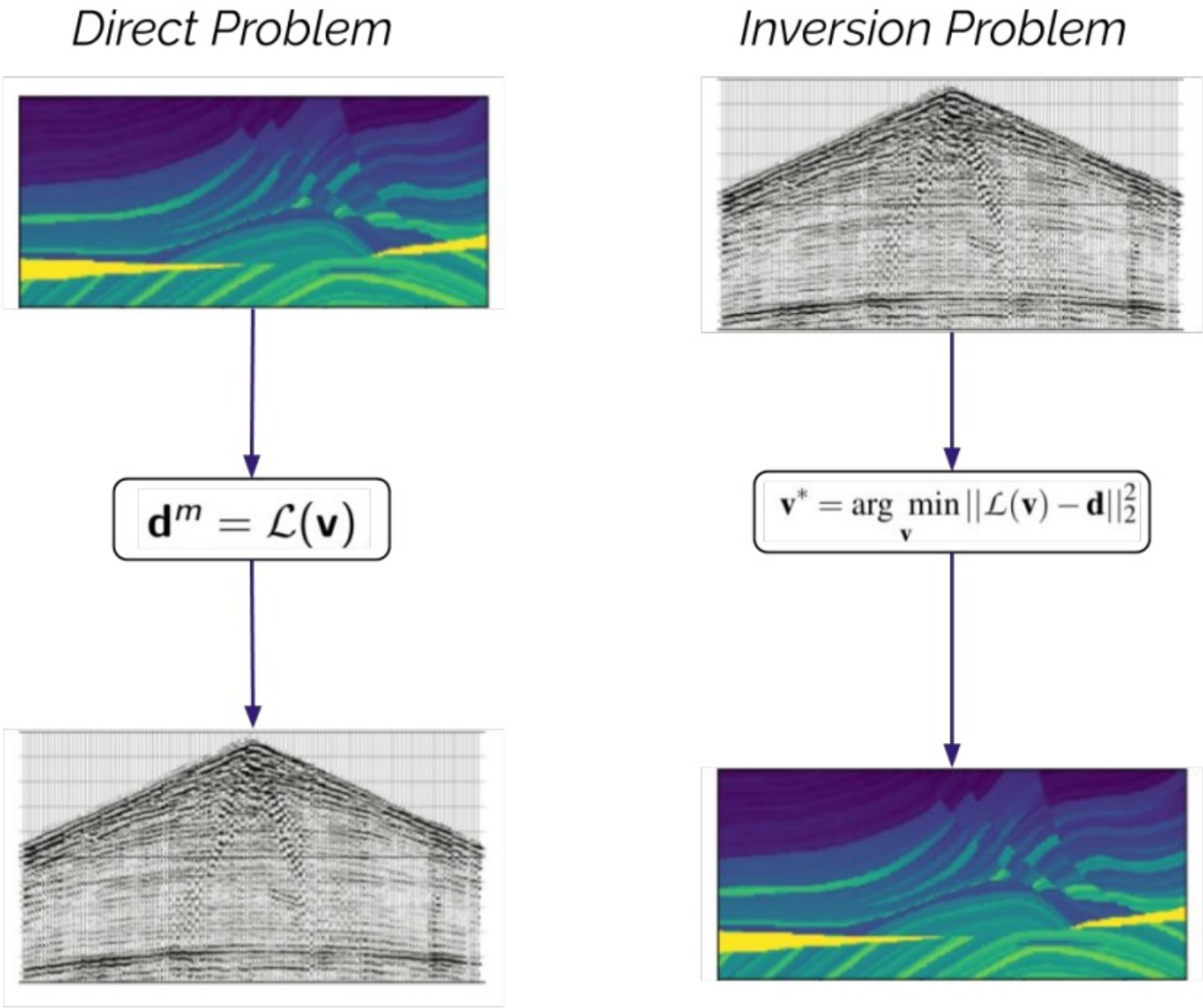
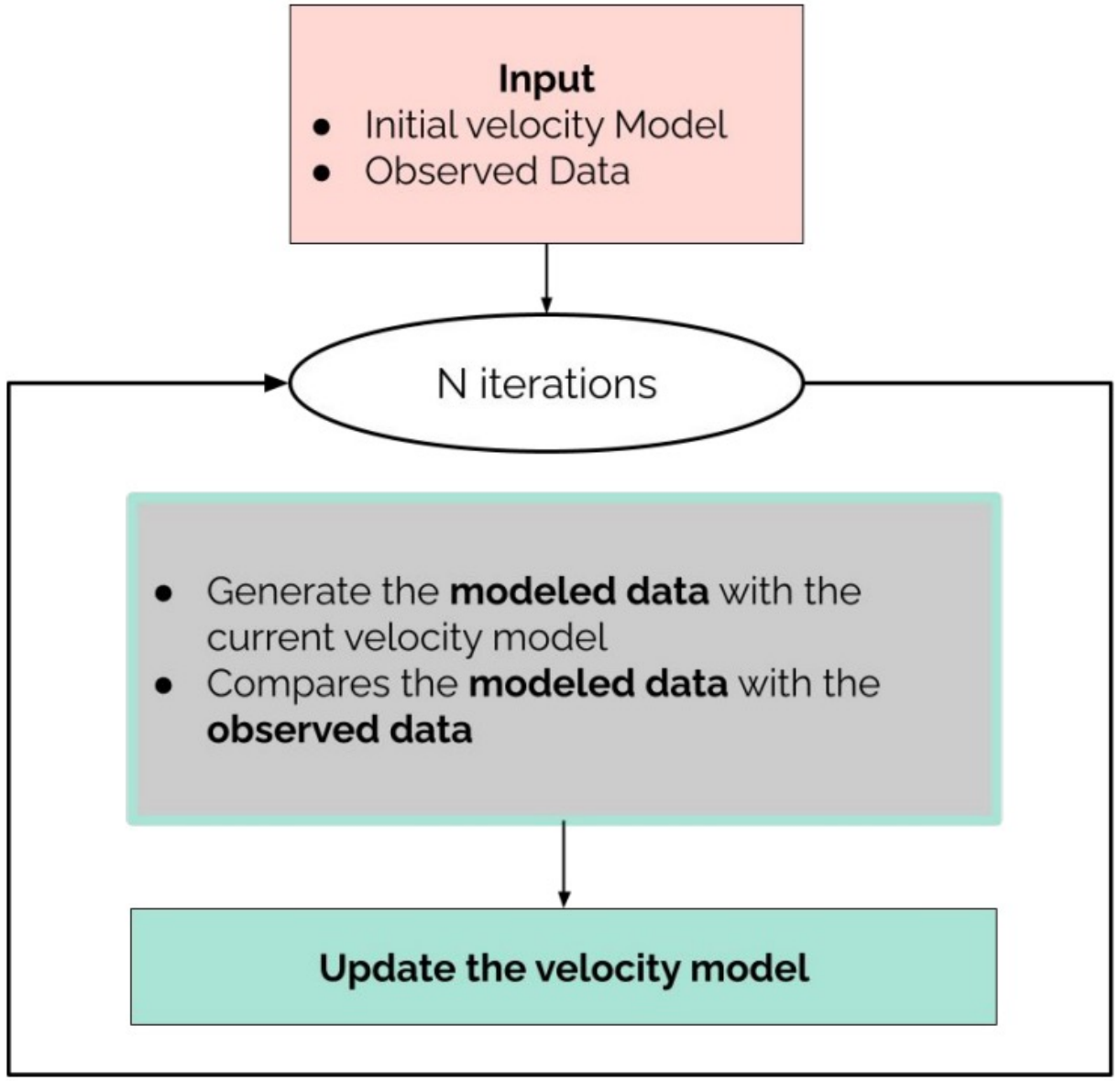


Figure from [7]

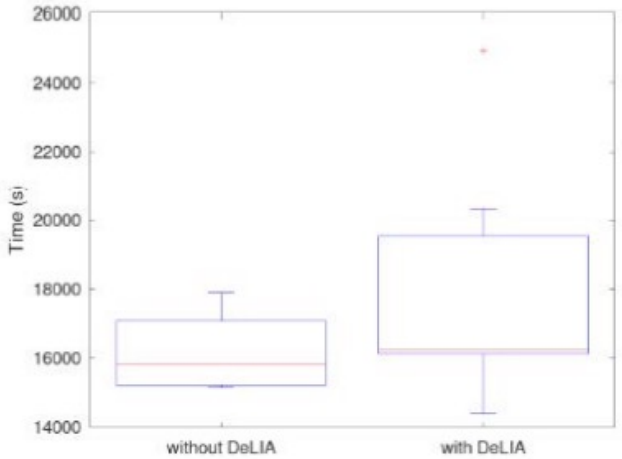
Case Study: 3D Full Waveform Inversion

Overview

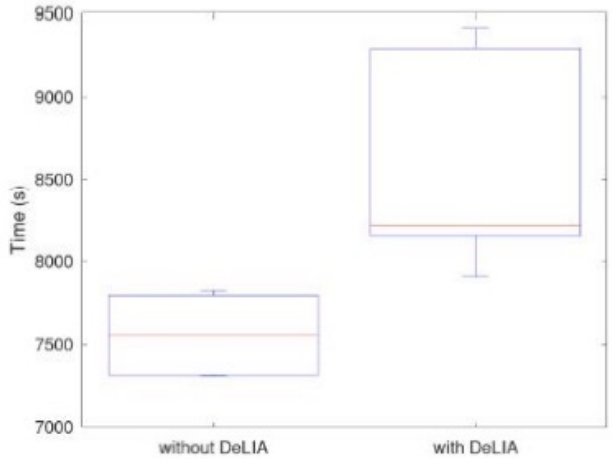


DeLIA in 3D FWI

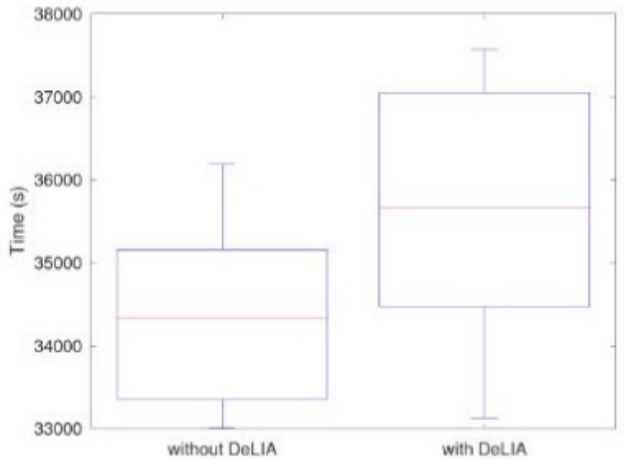
Experiments



Using four nodes 8 shots (a)



Using eight nodes 8 shots (b)



Using eight nodes 32 shots (b)

	4 nodes 8 shots	8 nodes 8 shots	8 nodes 32 shots
DeLIA overhead	2.54%	8.8%	3.84%
RSD without DeLIA	6.88%	3.37%	3.78%
RSD with DeLIA	17.40%	7.20%	5.14%

DeLIA Usability

- DeLIA provides an API to programmers to use the features in their software;
- The main parameters for DeLIA are defined by the developer in a JSON file.
- The library and its documentation are available at https://lappsufrn.gitlab.io/delia.

```
{
    "FT_FOLDER" : "./projects/fault_tolerance/data",
    "CHECKPOITING_GLOBAL_ITERATION": 1,
    "TRIGGER_SIGNAL" : true,
    "CHECKPOITING_TIME_GLOBAL": 60,
    "CHECKPOITING_TIME_LOCAL" : 10,
    "TRIGGER_HEARTBEAT_MONITORING": {
        "TIME_MAX_WAIT" : 60,
        "SLEEP_THREAD_TIME" : 5
    }
}
```

Next Steps

- Checkpoint with compressed data.
- The process shares encoded pieces of local data with more than one process. If one piece is lost, the other can reconstruct all data using the Reed-Solomon technique [6].
- Portability to other languages (e.g., python).

Thank you for your time

References

[1] Chetan S, A. Ranganathan, and R. Campbell. Towards fault tolerance pervasive computing. IEEE Technology and Society Magazine, 24(1):38–44, 2005.

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[3] de Haan, Dick, et al. Potential effects of seismic surveys on harbour porpoises. No. C126/15. IMARES, 2015.

[4] Herault T. and Robert Y. Fault-tolerance techniques for high-performance computing. Springer, 2015.

[5] Kalaiselvi S. and Rajaraman V.. A survey of checkpointing algorithms for parallel and distributed computers. Sadhana, 25(5):489–510, 2000.

[6] Reed, Daniel A., and Celso L. Mendes. "Reliability challenges in large systems." Future Generation Computer Systems 22.3 (2006): 293-302.

[7] Silva, Suzane Adrielly. Análise qualitativa do método de inversão completa das formas de onda no domínio do tempo. BS thesis. Universidade Federal do Rio Grande do Norte, 2017.

[8] Stephen B. Wicker and Vijay K. Bhargava. Reed-Solomon codes and their applications. John Wiley & Sons, 1999.

UNIVERSITY OF CAMBRIDGE

Fairy WANDS for Fusion

Stefanie Reuter[1], Jonathan Hollocombe[2], Toby James[2]

[1]Research Computing Services, UIS, University of Cambridge, UK
[2]UK Atomic Energy Authority

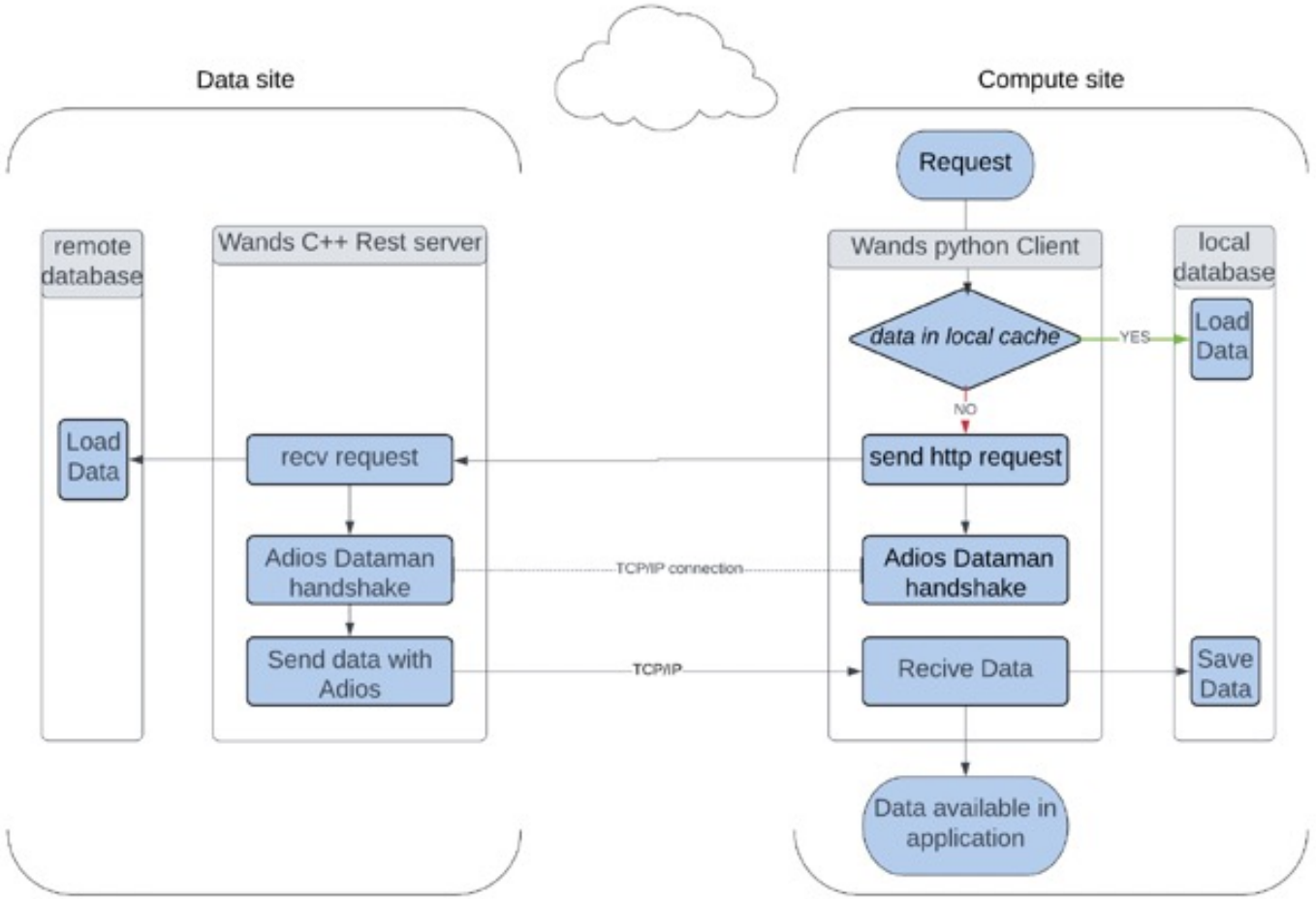
Women in HPC Poster Competition

Fairy WANDS for Fusion

Illustration of JET fusion tokamak reactor
(Credit: EUROfusion)

Cambridge Service for Data Driven Discovery
(Credit: Joe Bishop)

Wide Area Network Data Streaming



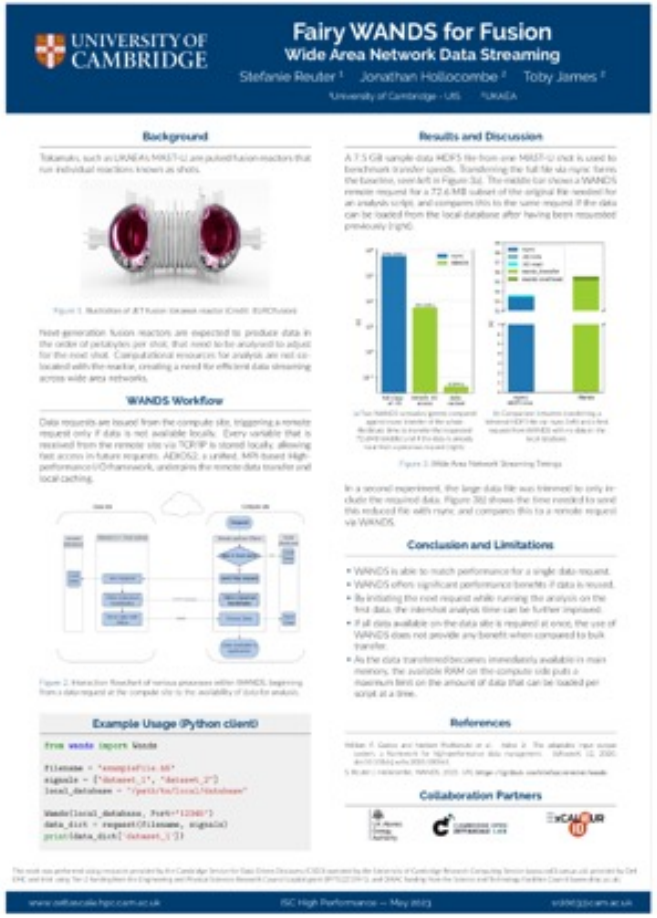
Python example usage

```
from wands import Wands

filename = "exampleFile.h5"
signals = ["dataset_1",
           "dataset_2"]
local_database = "/path/to/local/database"

wo = Wands(local_database,Port="12345")
data_dict = wo.request(filename,signals)

#do whatever you want with the data
```

Note: .h5 in remote database and .bp in local database

Thank you for your attention

Results?!? ⇒



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Fairy WANDS for Fusion

Wide Area Network Data Streaming

Stefanie Reuter [1] Jonathan Hollocombe [2] Toby James [2]

[1]University of Cambridge - UIS [2]UKAEA

Background

Tokamaks, such as UKAEA's MAST-U, are pulsed fusion reactors that run individual reactions known as shots.

Figure 1: Illustration of JET fusion (plasma) reactor (Credit: EUROfusion)

Next-generation fusion reactors are expected to produce data in the order of petabytes per shot, that need to be analysed to adjust for the next shot. Computational resources for analysis are not co-located with the reactor, creating a need for efficient data streaming across wide area networks.

WANDS Workflow

Data requests are issued from the compute site, triggering a remote request only if data is not available locally. Every variable that is received from the remote site via TCP/IP is stored locally, allowing fast access in future requests. ADIOS2, a unified, MPI-based High-performance I/O framework, underpins the remote data transfer and local caching.

Figure 2: Interaction flowchart of various processes within WANDS, beginning from a data request at the compute site to the availability of data for analysis.

Example Usage (Python client)

```
from wands import Wands

filename = "exampleFile.h5"
signals = ["dataset_1", "dataset_2"]
local_database = "/path/to/local/database"

Wands(local_database, Port="12345")
data_dict = request(filename, signals)
print(data_dict['dataset_1'])
```

Results and Discussion

A 7.5 GB sample data MDF5 file from one MAST-U shot is used to benchmark transfer speeds. Transferring the full file via rsync forms the baseline, seen left in Figure 3a). The middle bar shows a WANDS remote request for a 72.6 MB subset of the original file needed for an analysis script, and compares this to the same request if the data can be loaded from the local database after having been requested previously (right).

Figure 3: Wide Area Network Streaming Timings

In a second experiment, the large data file was trimmed to only include the required data. Figure 3b) shows the time needed to send this reduced file with rsync and compares this to a remote request via WANDS.

Conclusion and Limitations

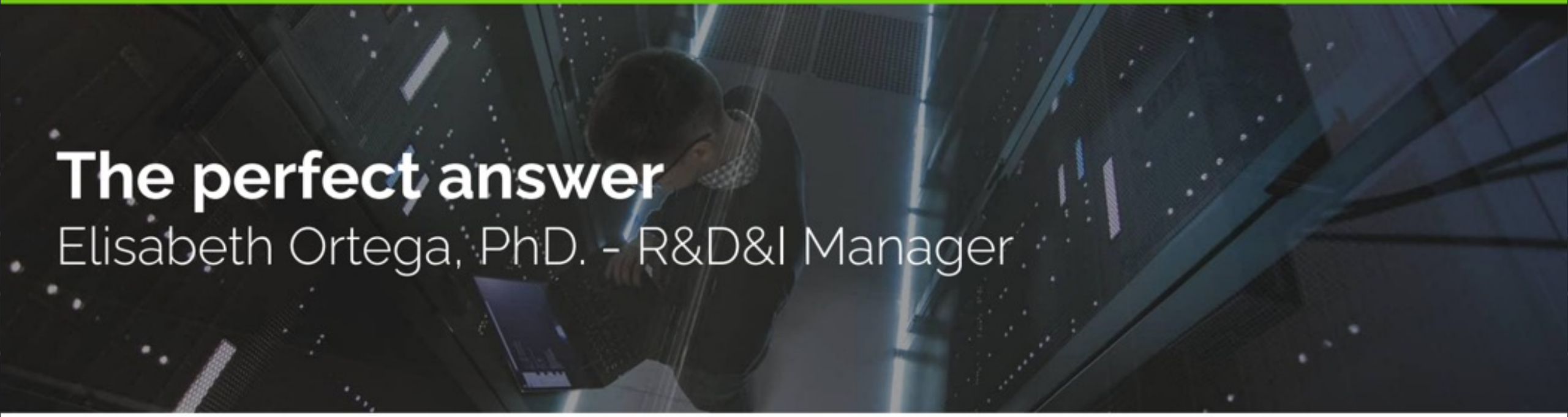
- WANDS is able to match performance for a single data request.
- WANDS offers significant performance benefits if data is reused.
- By initiating the next request while running the analysis on the first data, the individual analysis time can be further improved.
- If all data available on the data site is required at once, the use of WANDS does not provide any benefit when compared to bulk transfer.
- As the data transferred becomes immediately available in main memory, the available RAM on the compute side puts a maximum limit on the amount of data that can be loaded per script at a time.

References

Collaboration Partners

This work was performed using resources provided by the Cambridge Service for Data Driven Discovery (CSD3) operated by the University of Cambridge Research Computing Service (www.csd3.cam.ac.uk), provided by Dell EMC and Intel using Tier-2 funding from the Engineering and Physical Sciences Research Council (capital grant EP/T022159/1), and DiRAC funding from the Science and Technology Facilities Council (www.dirac.ac.uk).

HPC Now!



The perfect answer

Elisabeth Ortega, PhD. - R&D&I Manager

22/05/2023

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ISC23 Exhibitor Forum - WHPC

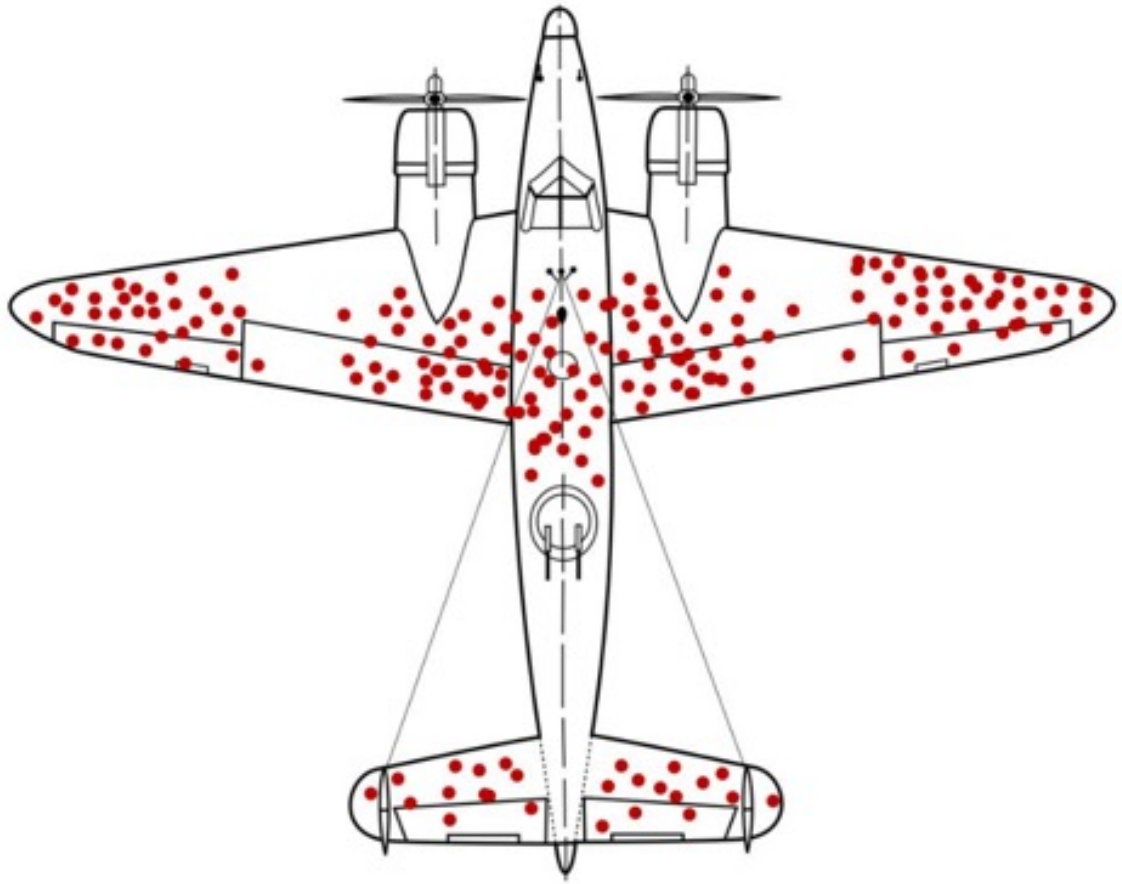
… for the question:

Image by studiogstock - Freepik

which I was not able to answer properly until I had a conversation with a woman in HPC at my early career in HPC (one year ago)

which I was not able to answer properly until I had a conversation with a woman in HPC at my early career in HPC (one year ago)

(which I'll answer with a story)

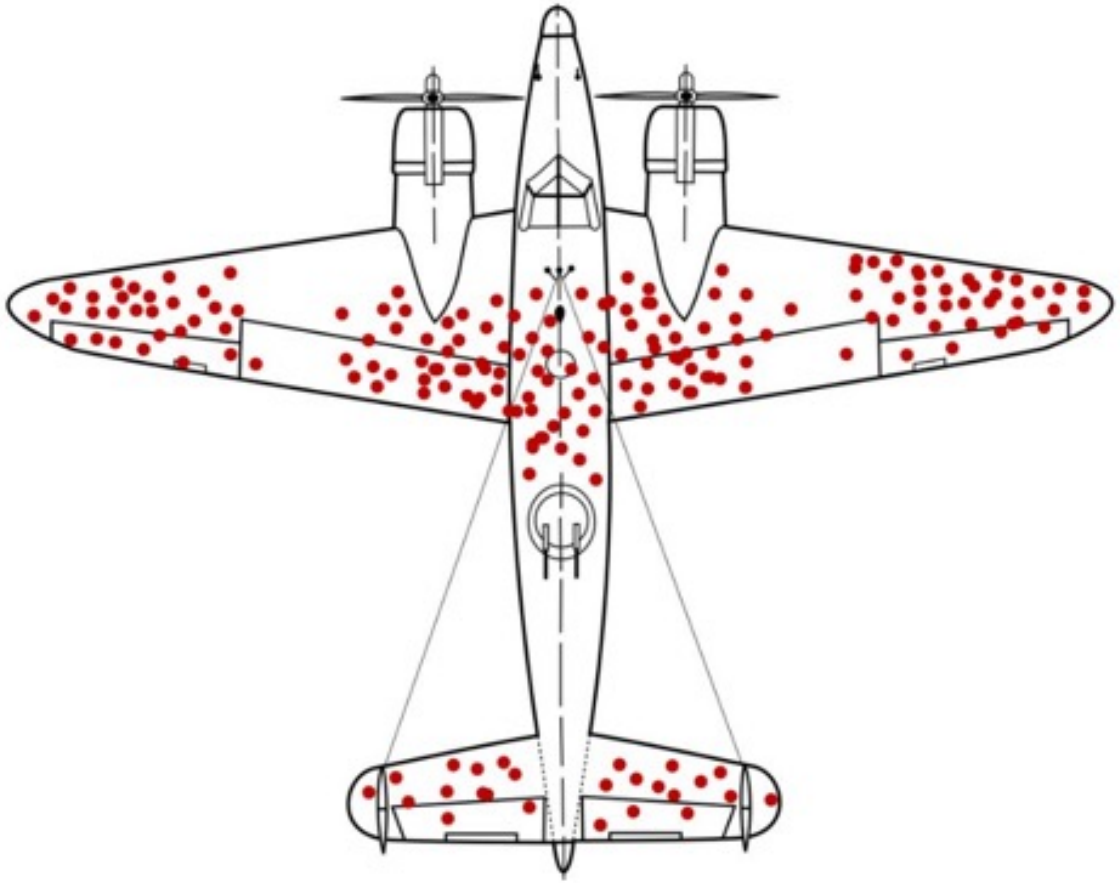


The topic:

Improving the durability of planes by adding extra pieces of metal on the critical parts of the plane considering the bullet hits of the returning planes, but where?

a) In the bullet holes (red dots)

b) In other places



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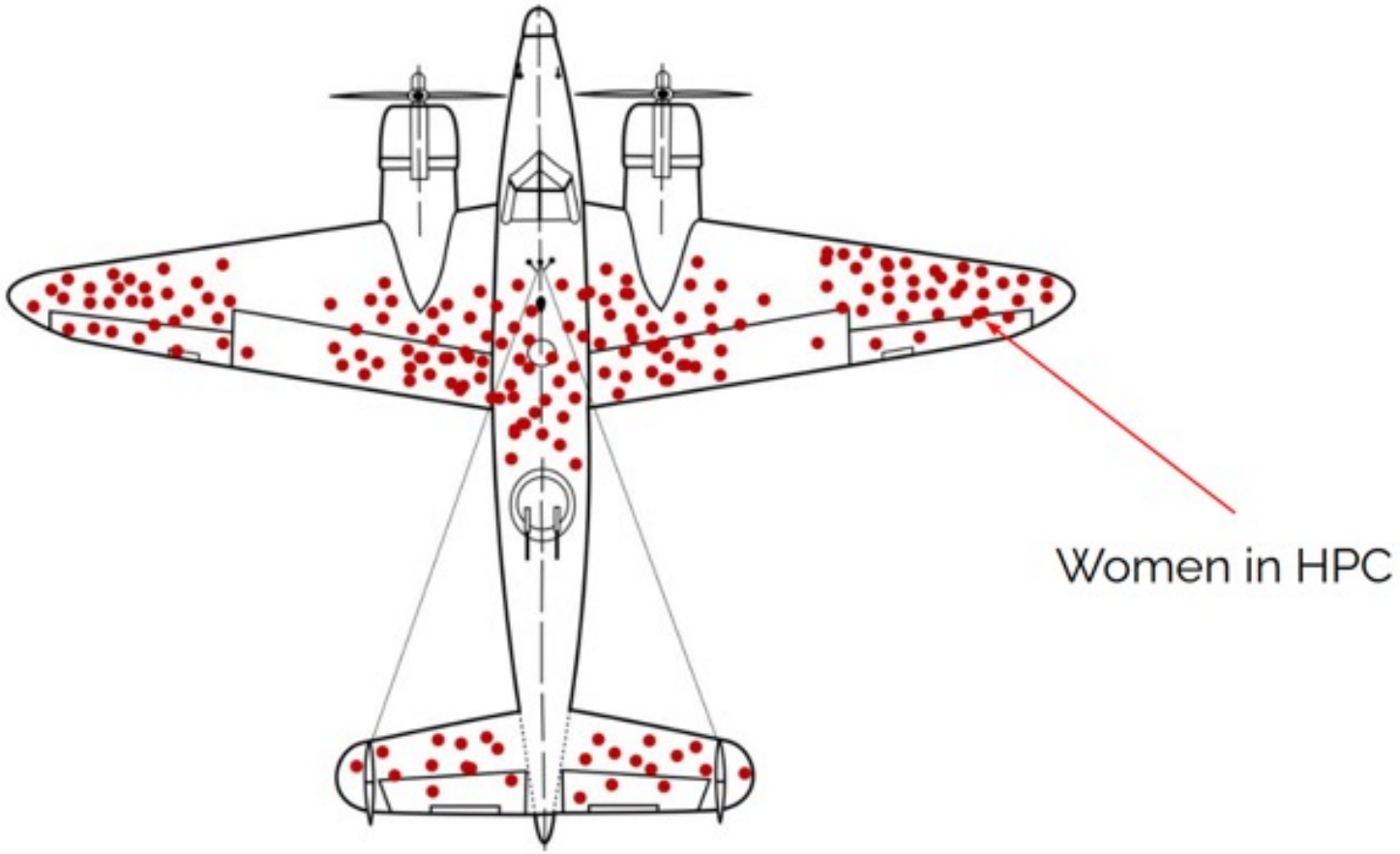
HPC Now!

It's not wrong data, it's the wrong approach



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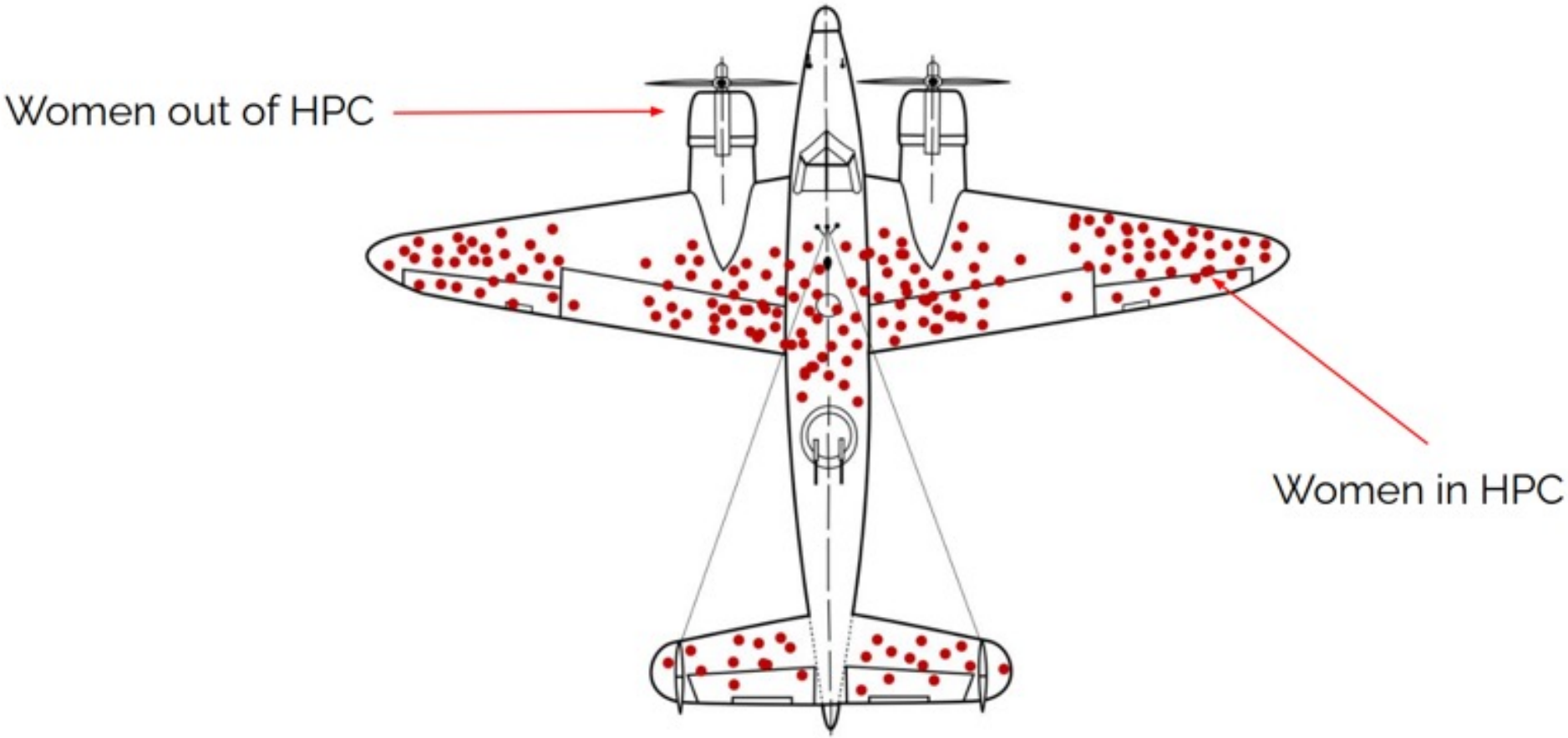


HPC Now!

The perfect answer is ...

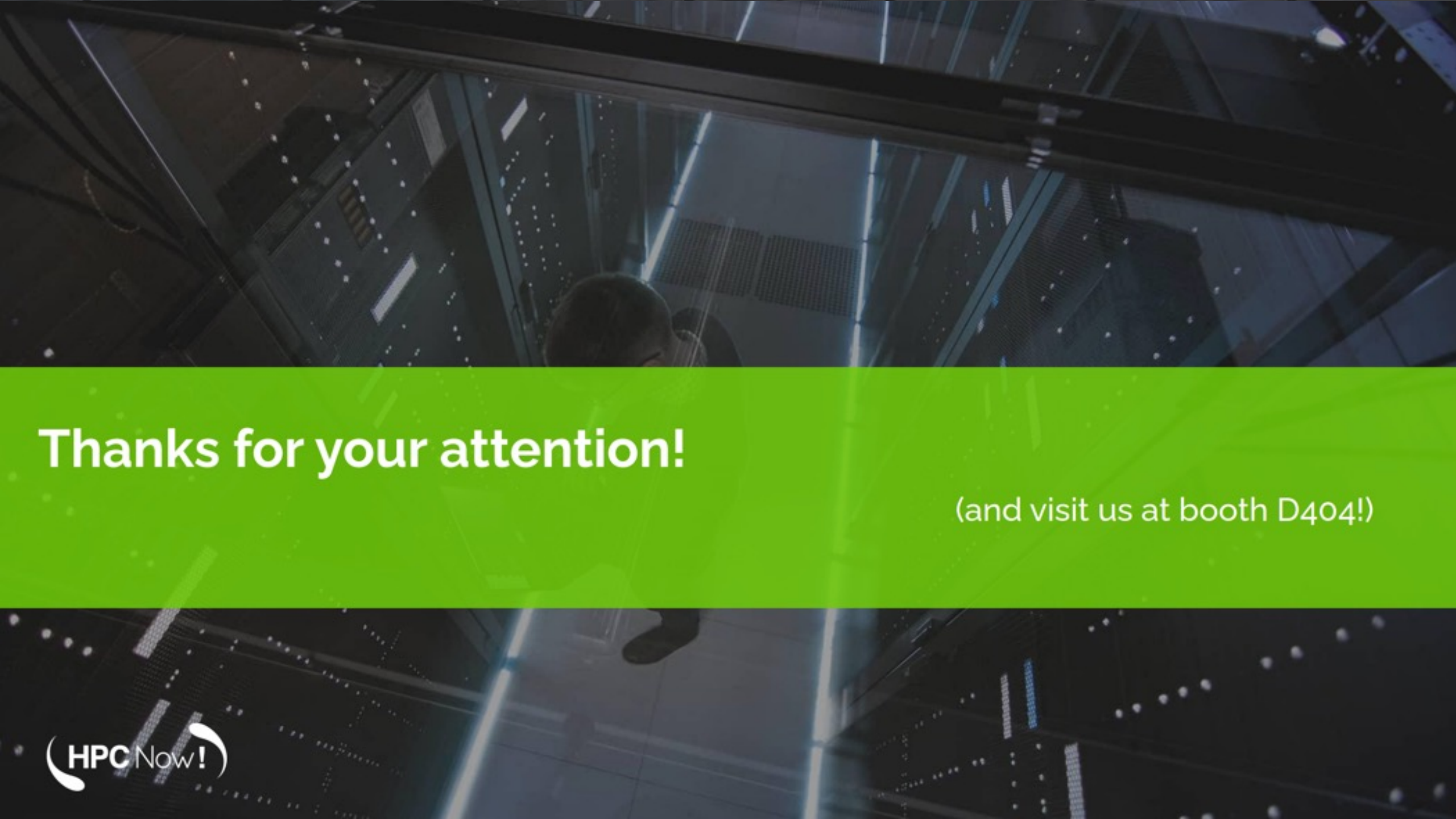
HPC Now!

The perfect answer is ...

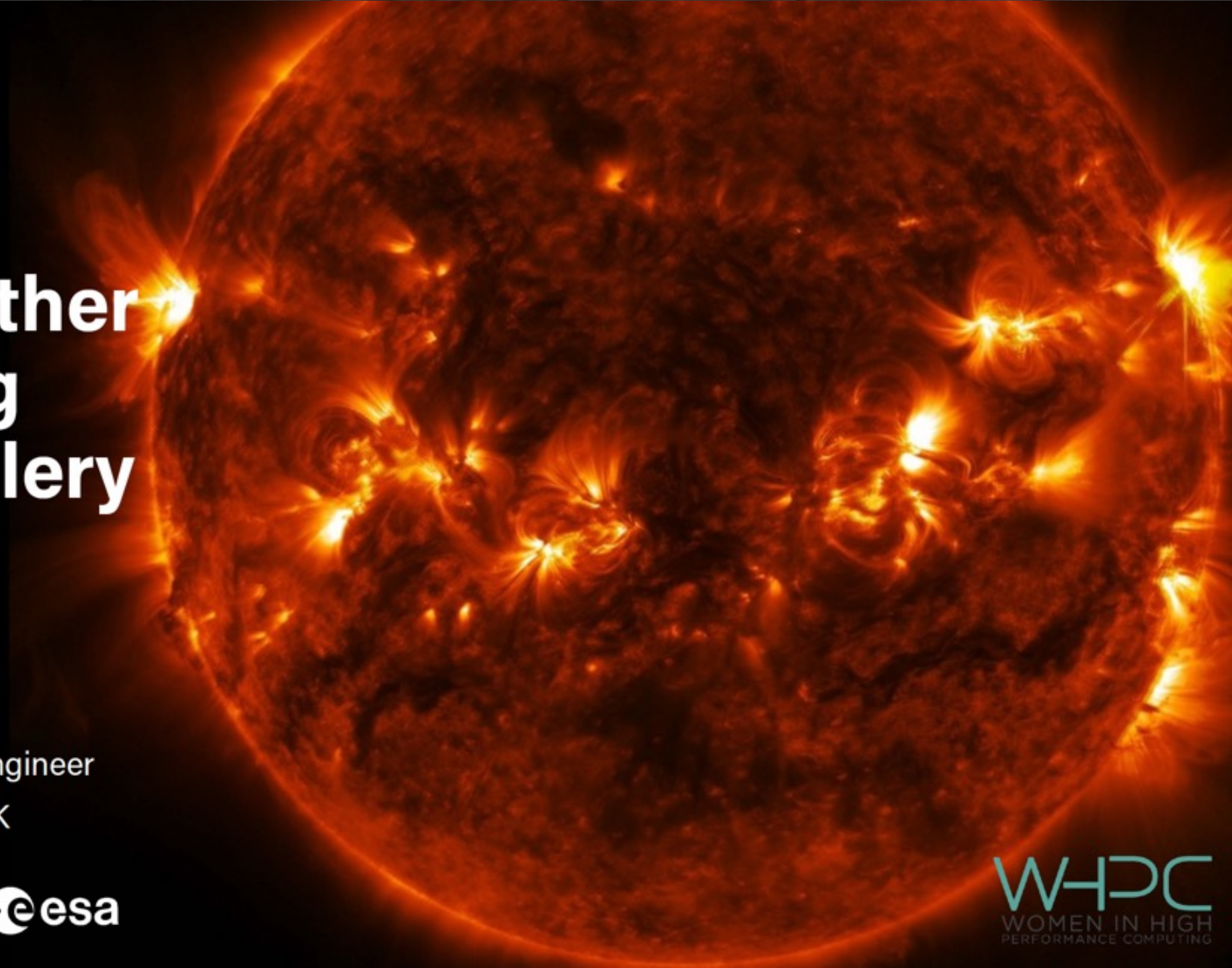
don't ask it to me

The perfect answer is ...

don't ask it to me


Thanks for your attention!
(and visit us at booth D404!)
HPC Now!

Space Weather Forecasting using Celery and django



Dr Jenny Wong

Senior Research Software Engineer

University of Birmingham, UK

UNIVERSITY OF BIRMINGHAM

SERENE SPACE ENVIRONMENT

esa

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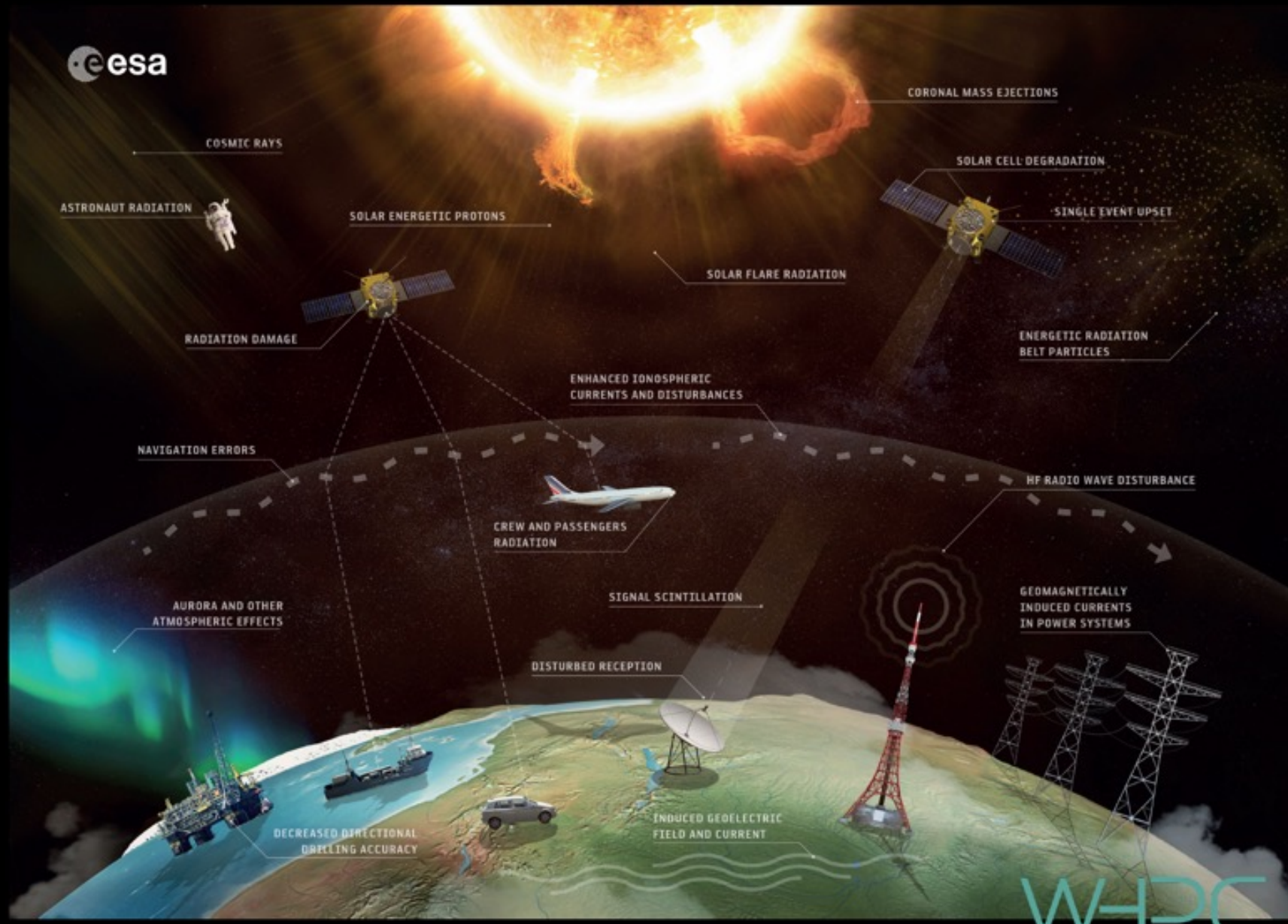
Space Weather Forecasting

- Forecasting space weather conditions in the Earth's ionosphere is critical to protecting key infrastructure
- Variations in space weather are caused by Coronal Mass Ejections from the Sun's surface
- Produces disturbances in communications and electrical systems, as well as spectacular aurorae



WHPC
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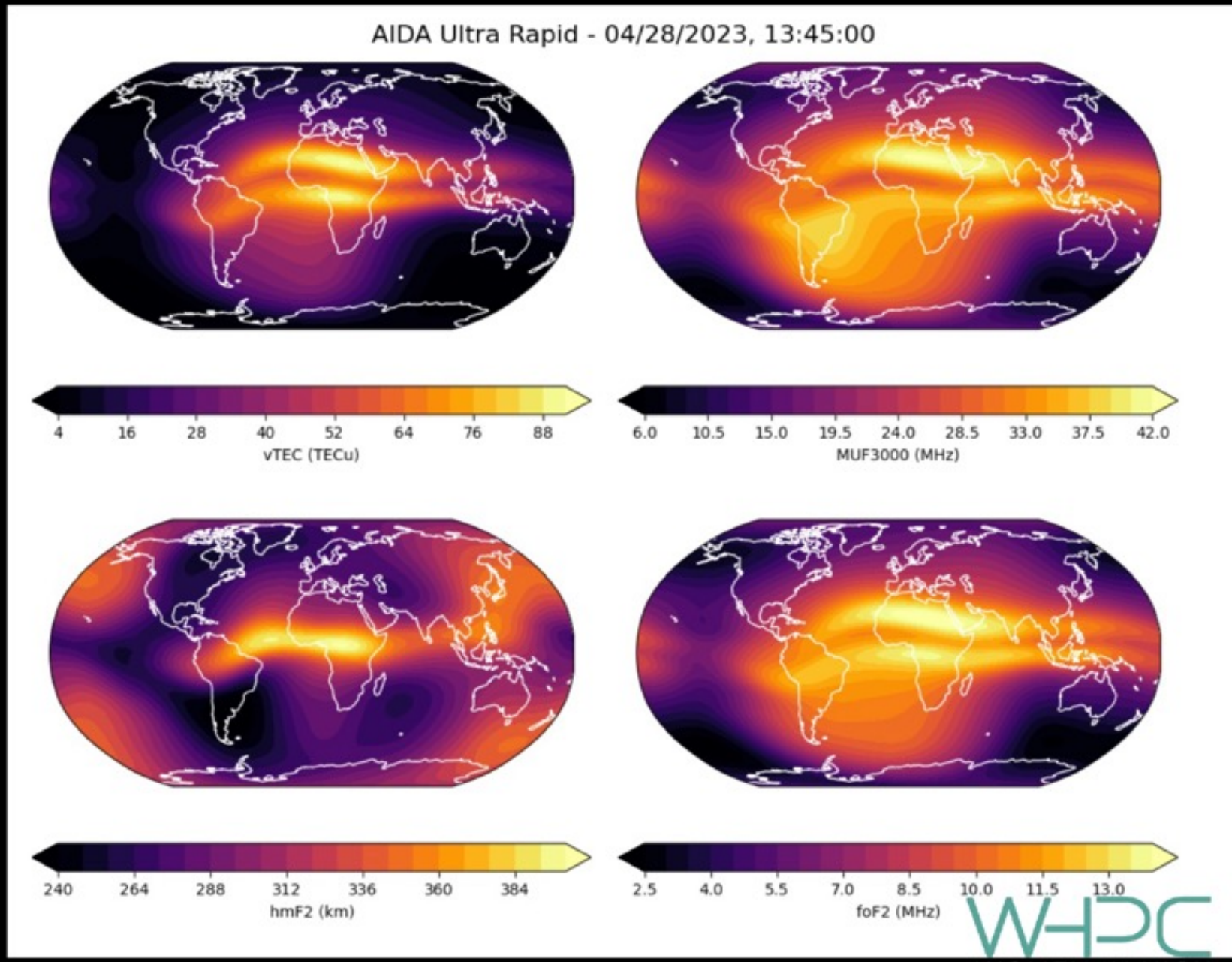
Making automated, HPC-powered scientific results accessible in near-real time

- We present a system for operationalising HPC tasks for data assimilation in space weather forecasting using Celery and Django
- Celery is a distributed task queue used to execute asynchronous jobs
- Django is popular Python-based web framework where simulation outputs are presented



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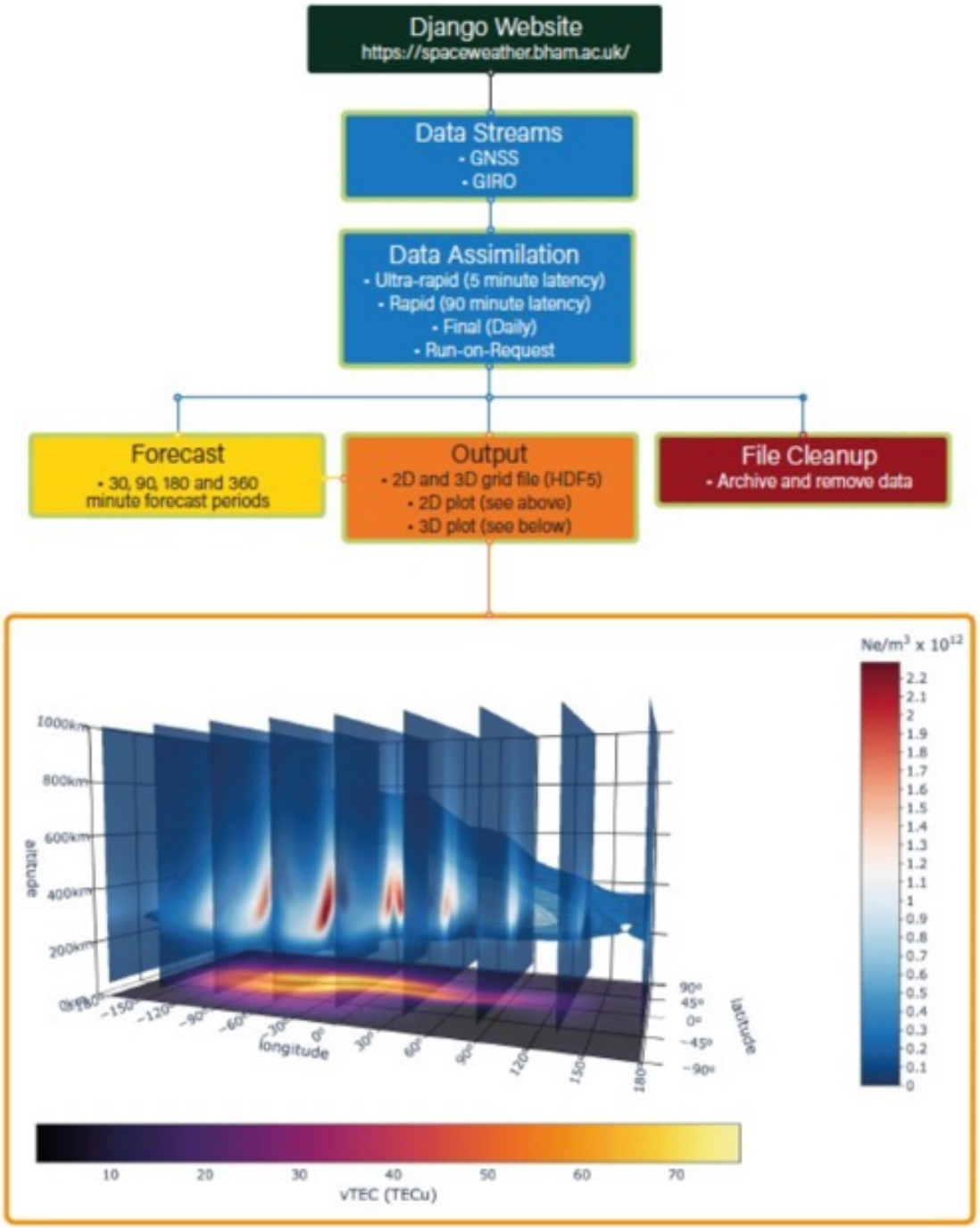

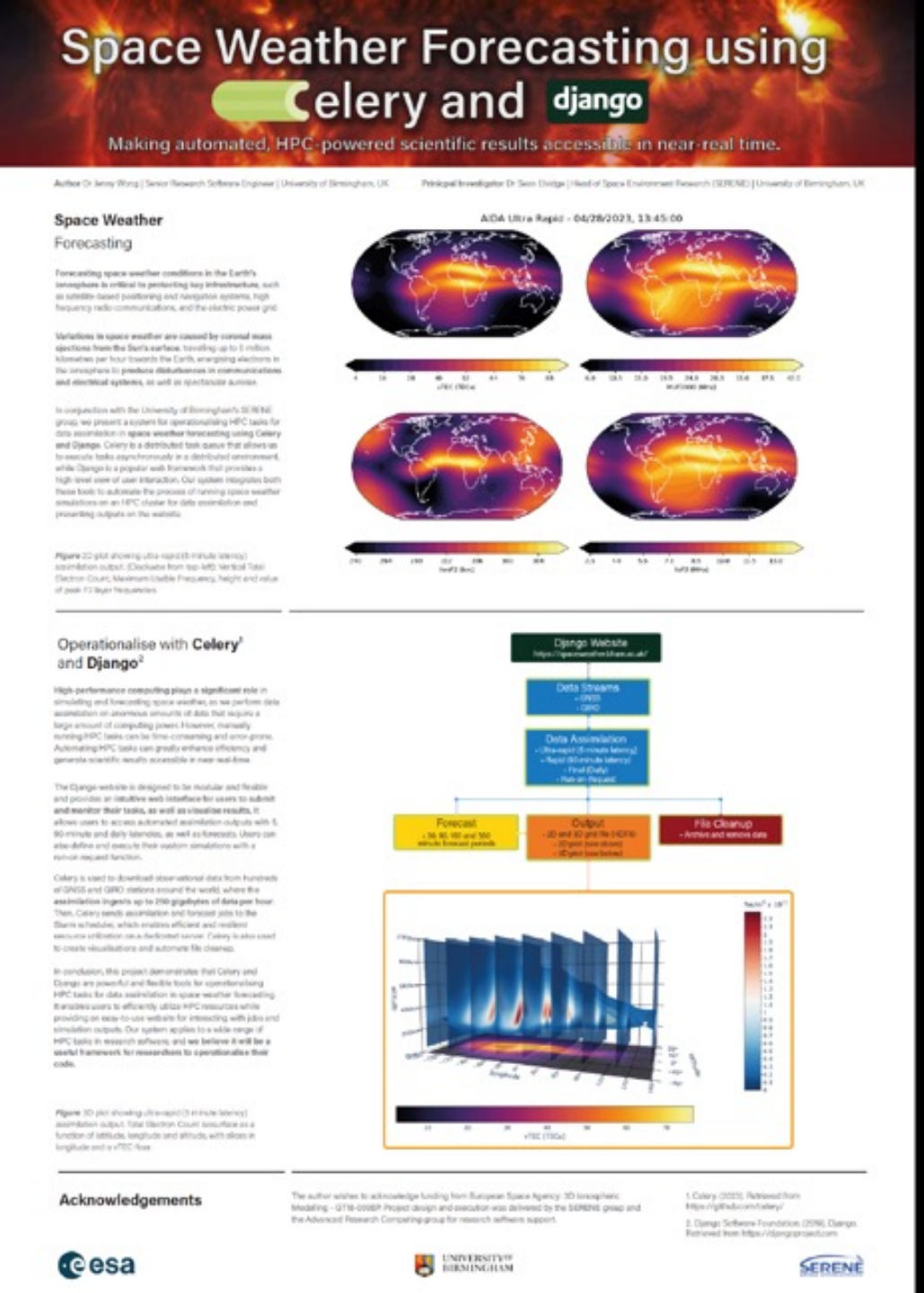

Space weather forecasting using Celery and Django: Making automated, HPC-powered scientific results accessible in near-real time.

Foyer D-G - 2nd Floor
Women in HPC Poster

Dr Jenny Wong
Senior Research Software Engineer
University of Birmingham, UK

@_jennywong_ thisisjennywong

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3:30 - 5:30 PM

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Women in HPC

Deb Goldfarb

Director of Product + Strategy
for HPC & Batch, AWS

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LESSONS

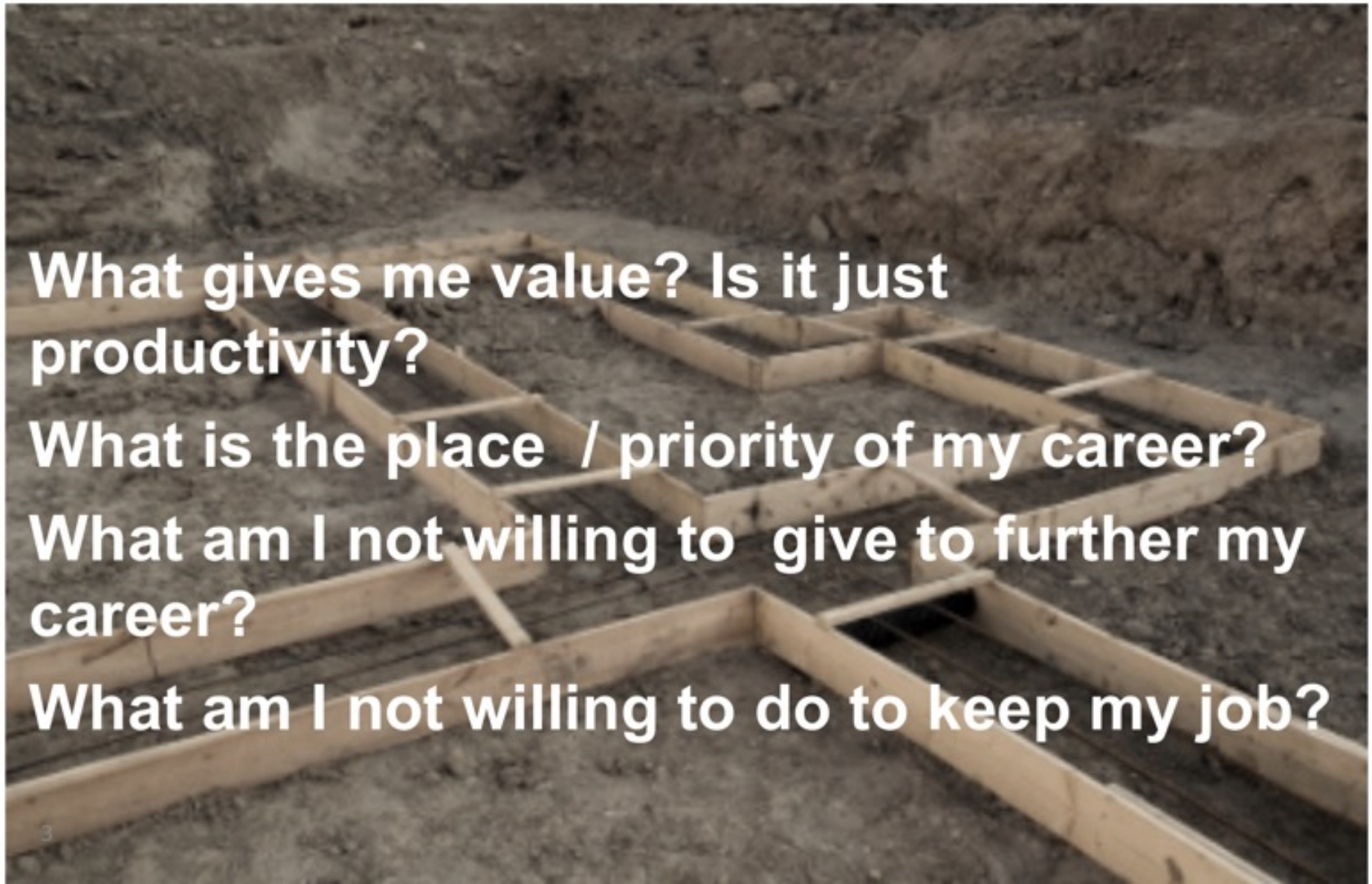
Stuff I learned along the way which turned out to be important

Debra Goldfarb
Director, HPC Products and Strategy, AWS

aws

Inspired by mistakes…
…My own and those of others

Lesson 1
…Laying a Foundation



Lesson 2
…Most of Us Have Impostor Syndrome

"It's perfectly okay to occasionally feel like a fraud when it comes to your career. I'm just not sure you need to say that on your resume."

Lesson 3
Do it anyway

Final Thoughts

Let your values drive your career

Don’t crush yourself with false expectations or comparisons

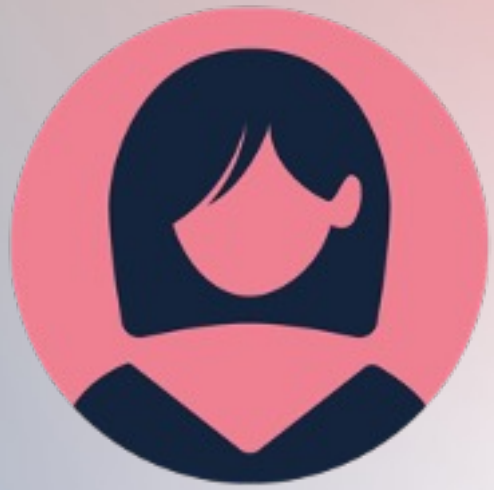
Ask for what you want…and deserve

Celebrate where you are

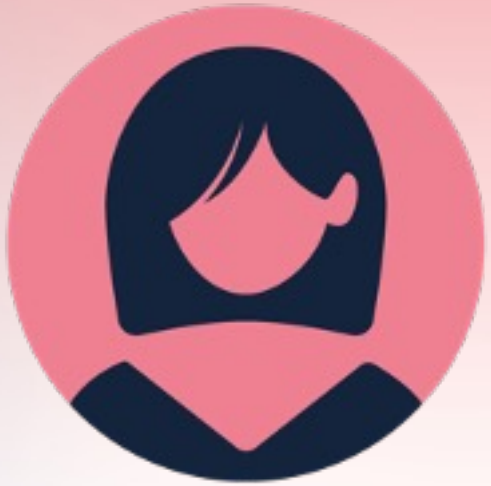
Early Career Speakers

Paula Esposito
La Laguna University

Aleksandra Kowalczuk
University of Warsaw



Ekaterina Zossimova
University of Exeter



Helena Vela Beltran
Barcelona Supercomputing Center

WHPC
WOMEN IN HPC

ISC High Performance
The HPC Event.

WHPC

Performance Analysis of Parallel Codes with FancyJCL

High Performance Computing Group
Department of Computer Engineering and Systems, University of La Laguna

Sergio Afonso
Óscar Gómez-Cárdenes
Paula Expósito
Vicente Blanco
Francisco Almeida

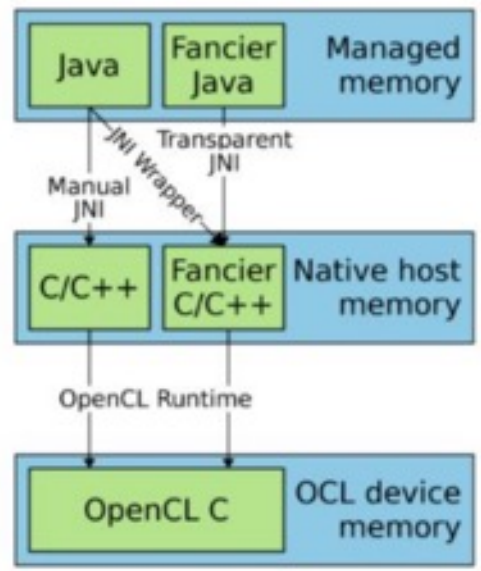
Universidad de La Laguna

Problematic of acceleration on mobile devices

The advances on SoC hardware are not up to par with the software's

Workflow for execute an app on a mobile device's GPU

Communication between memory spaces



FancyJCL

Through a sequential interface users can accelerate applications

FancyJCL is built on the top of the Fancier library for avoiding memory copies

Adding a constant to an array with FancyJCL

```
public class Foo {
    public void run (long[] array, long kConstant) {
        Stage stage = new Stage();
        stage.setKernelSource("array[d0] += kConstant;");
        stage.setInputs(Map.of("array", array, "kConstant", kConstant));
        stage.setOutputs(Map.of("array", array));
        stage.setRunConfiguration(new RunConfiguration(new long[]{array.length},
                                                       new long[]{4}));
        stage.runSync();
    }
}
```

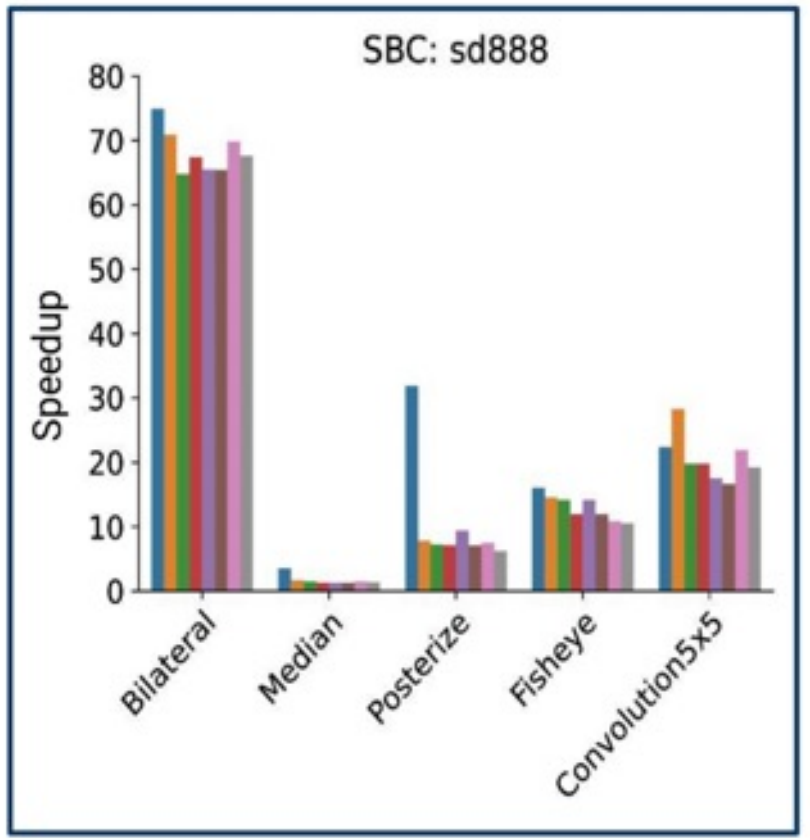
Results

Algorithms

x5 Image Processing Algorithms
x8 Different Image Resolution

Devices

Device	System-on-Chip	Characteristics
Xiaomi Mi Mix 2	Snapdragon 845	Programmable GPU Unified Memory Architecture
Snapdragon 865 SDK	Snapdragon 865	
Vivo iQOO 7	Snapdragon 888	



In horizontal, 5 groups of kernels with 8 resolutions each. In vertical, achieved speedup.

Thank you for your attention

Sergio Afonso	safonsof@ull.edu.es
Óscar Gómez-Cárdenes	ogomezca@ull.edu.es
Paula Expósito	**pexposit@ull.edu.es**
Vicente Blanco	vblanco@ull.edu.es
Francisco Almeida	falmeida@ull.edu.es

Acknowledgements: This work has been supported by the Spanish Ministry of Science and Innovation with the PID2019-107228RB-I00, TED2021-131019B-I00 and PDC2022-134013-I00 projects; and by the Government of the Canary Islands with the project ProID2021010012.

GOBIERNO DE ESPAÑA · MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

Gobierno de Canarias
Consejería de Economía, Industria, Comercio y Conocimiento
Agencia Canaria de Investigación, Innovación y Sociedad de la Información

Universidad de La Laguna

CAPAP-H

ISC HIGH PERFORMANCE, HAMBURG 2023

APPLICATION OF ADVANCED TEXT ANALYSIS IN THE STUDY OF SCIENTIFIC LITERATURE

ALEKSANDRA KOWALCZUK
INTERDISCIPLINARY CENTRE FOR MATHEMATICAL AND COMPUTATIONAL MODELLING

UNIVERSITY OF WARSAW
Interdisciplinary Centre for Mathematical and Computational Modelling
icm.edu.pl

OUTLINE

- Background
- State of Art
- Methods
- Preliminary Results
- The Future

BACKGROUND

In view of the constantly growing amount of scientific literature, there is a real need to make it easier for experts like medical doctors to access resources published around the world and quickly draw conclusions from them.

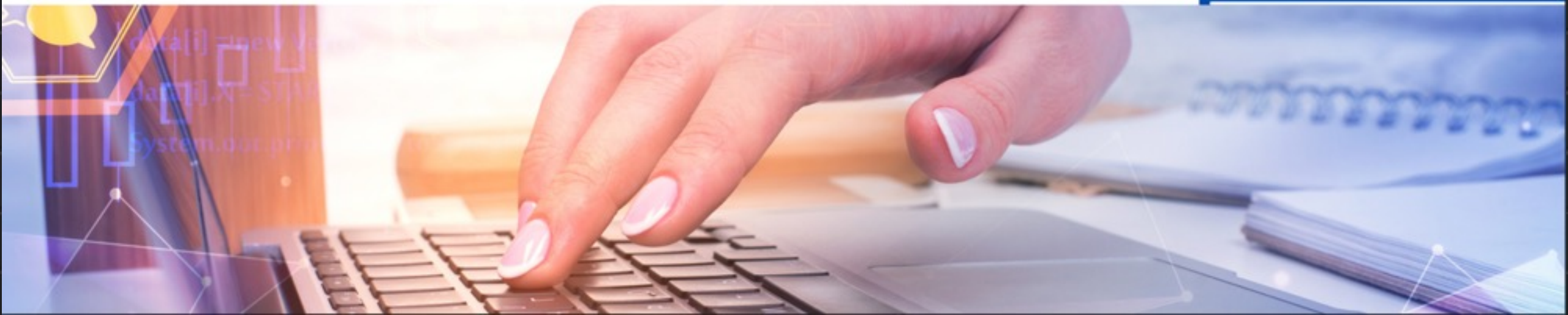
What is the Value?

Discovery of novel tools

Identification of promising new paths in science

Better performance of research organisations

Improvement of career paths for researchers



STATE OF ART

We can observe a very dynamic development of AI natural language models and ready-to-use tools dedicated to text analysis, processing and generation.

Challenges

Different scientific data formats

Accessing and searching relevant scientific literature

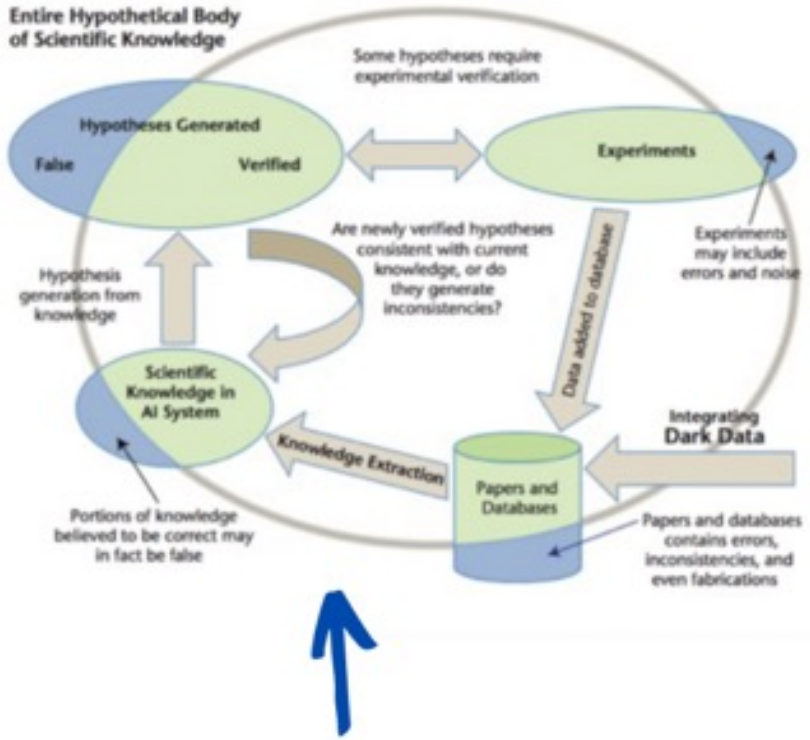
The direction of valuable research work

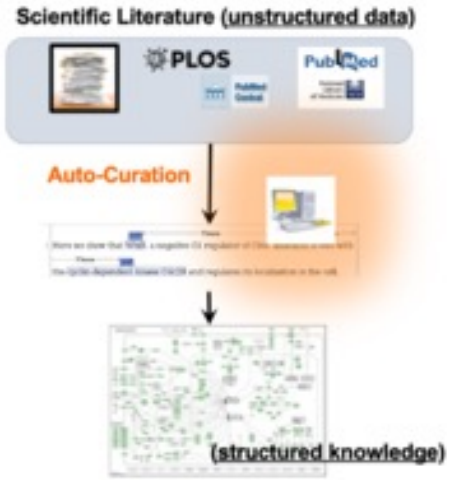
More and more advanced language models for NLP

Hardware and computing power

Scientific, social and legal impact

METHODS

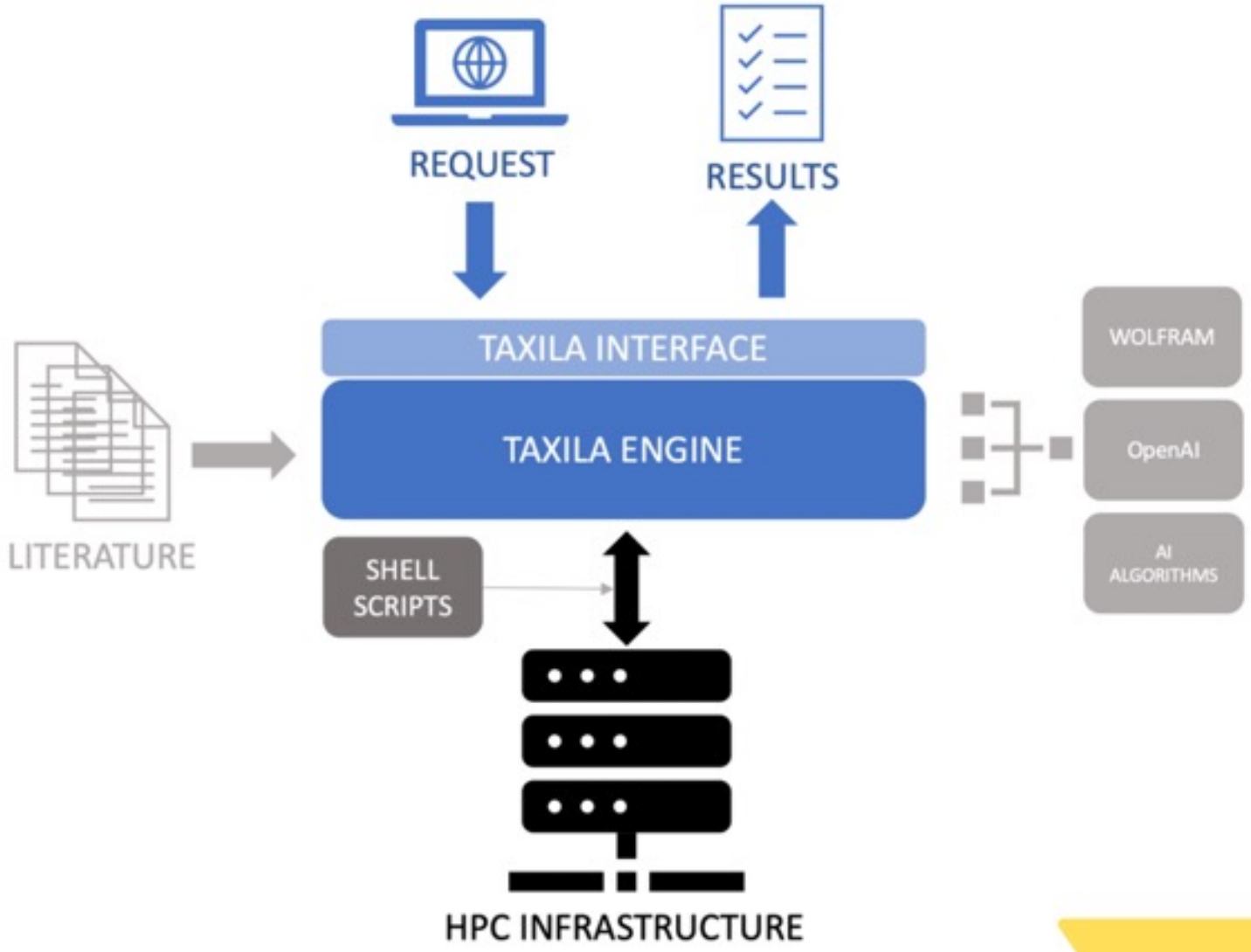




- Engine of scientific discovery: Taxila
- Intelligent algorithms and scripts: language models for NLP
- Ready-to-use tools: OpenAI, Wolfram
- Analyzing text in biological context: CAR-T therapy

Source: SBI Poland Workshops 2021 - Taxila

ARCHITECTURE



PRELIMINARY RESULTS

THE FUTURE

Can a machine write a good scientific article?
Can a machine win the Nobel Prize?

"Our ultimate goal is to develop an AI System that can make major scientific discoveries that would improve the state of the world and impacting the way we do science."

Hiraoki Kitano, SBI Tokyo

SOURCES

[1] Taxila Curation

https://curation.taxila.io

[2] SBI Publications

https://medium.com/@sbijapan

[3] OpenAI

https://openai.com

[4] Wolfram Alpha Series of Articles

https://writings.stephenwolfram.com

[5] T-PAIR: Temporal Node-pair Embedding for Automatic Biomedical Hypothesis Generation

IEEE XPLORE, Vol. 34 Issue: 6

Uchenna Akujuobi, Michael Spranger, Sucheendra K. Palaniappan, Xiangliang Zhang

[6] What Is ChatGPT Doing ... and Why Does It Work?

Wolfram Research, Inc., March 2023

Stephen Wolfram

THANK YOU!

ALEXANDRA.KOWALCZUK@GMAIL.COM

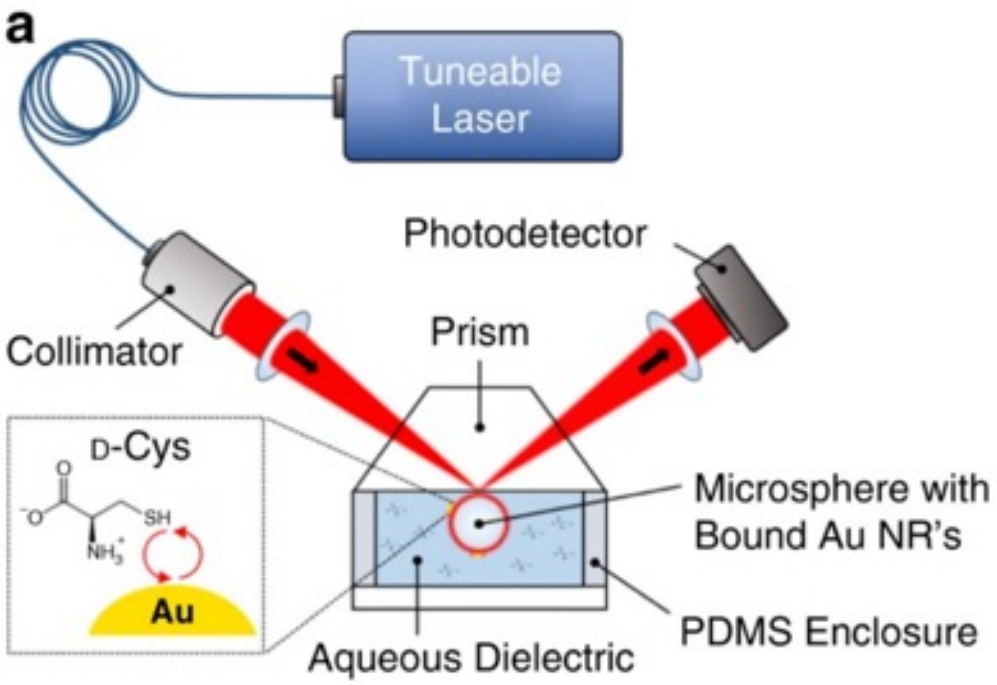
High Performance Computing for Decoding Biosensor Signals

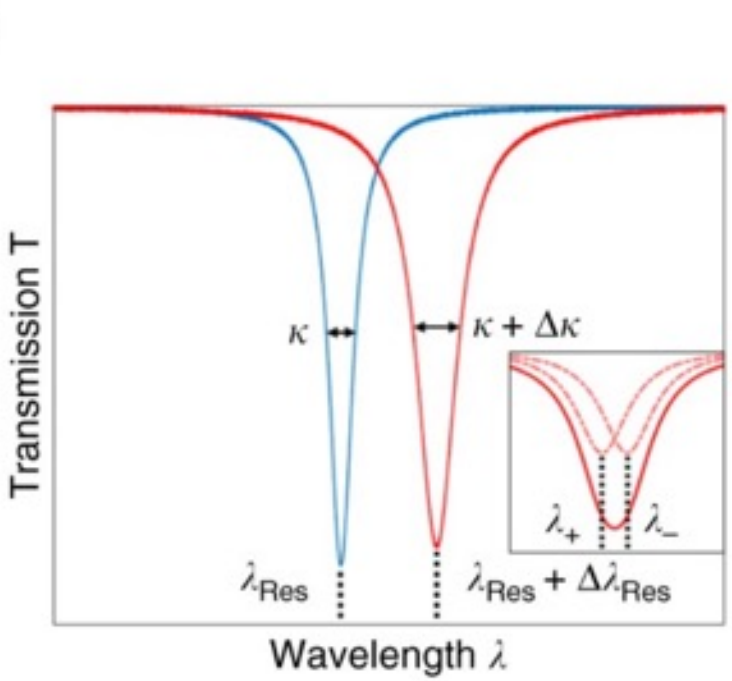
Ekaterina Zossimova and Michael Walter

University of Exeter, UK & Freiburg Center for Interactive Materials and Bioinspired Technologies, Germany

22 May 2023

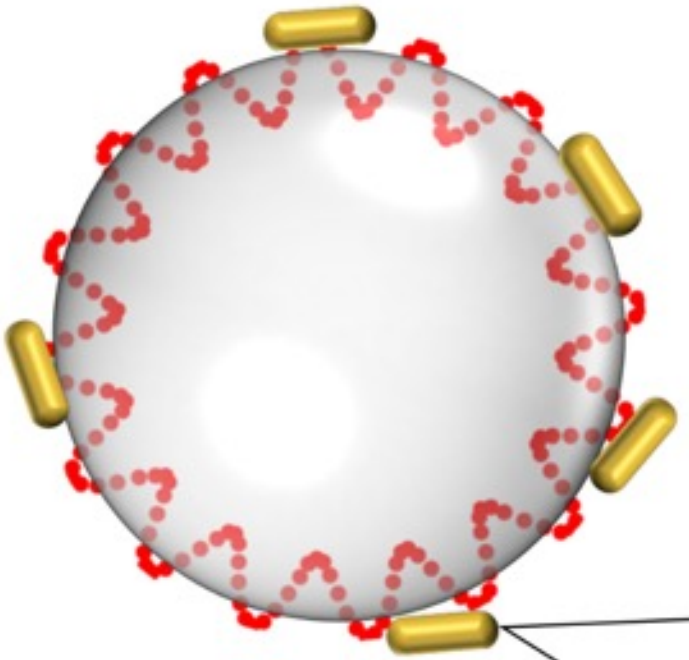
Opto-plasmonic biosensor

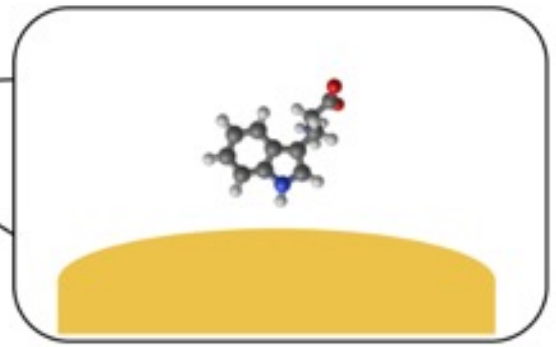




Vincent, S., Subramanian, S. & Vollmer, F. Optoplasmonic characterisation of reversible disulfide interactions at single thiol sites in the attomolar regime. Nat Commun 11, 2043 (2020). Licensed under Creative Commons CC BY

Opto-plasmonic biosensor





Excess polarizability (from electronic structure calculations)

Wavelength shift

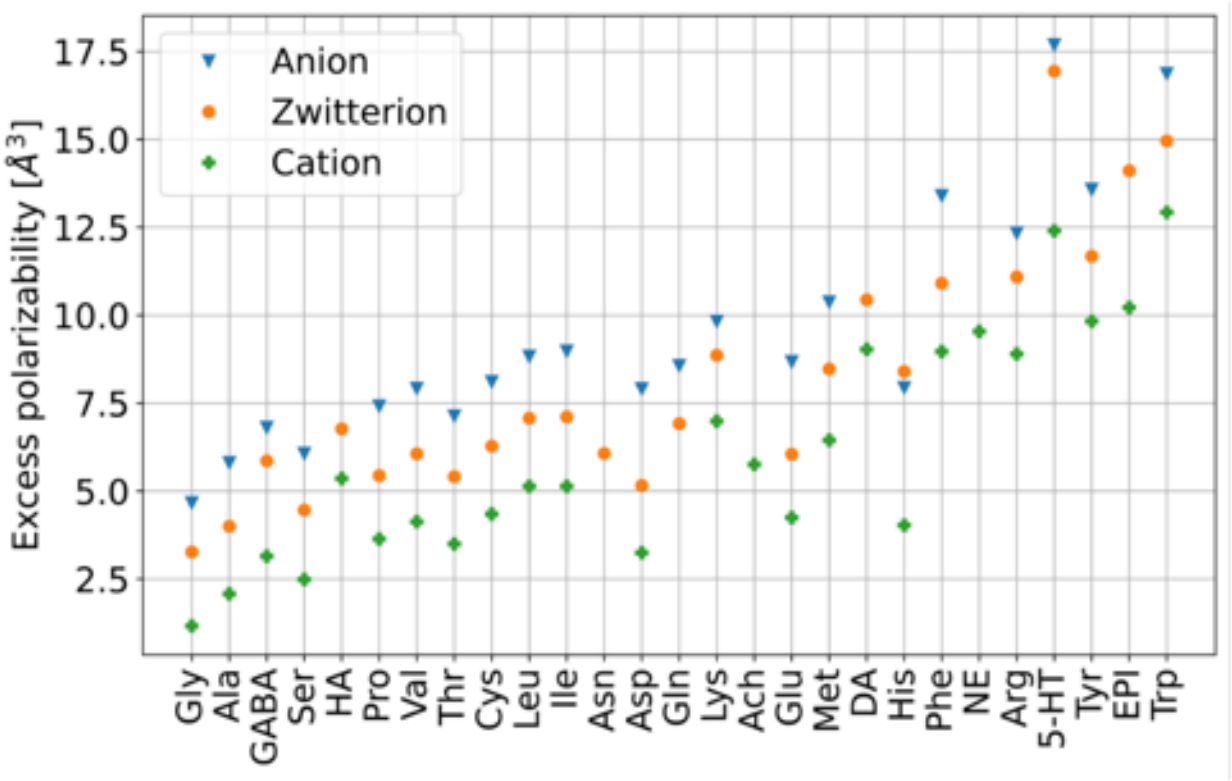
$$\frac{\Delta\lambda}{\lambda_0} = \frac{\alpha_{ex}}{2V_{eff}}$$

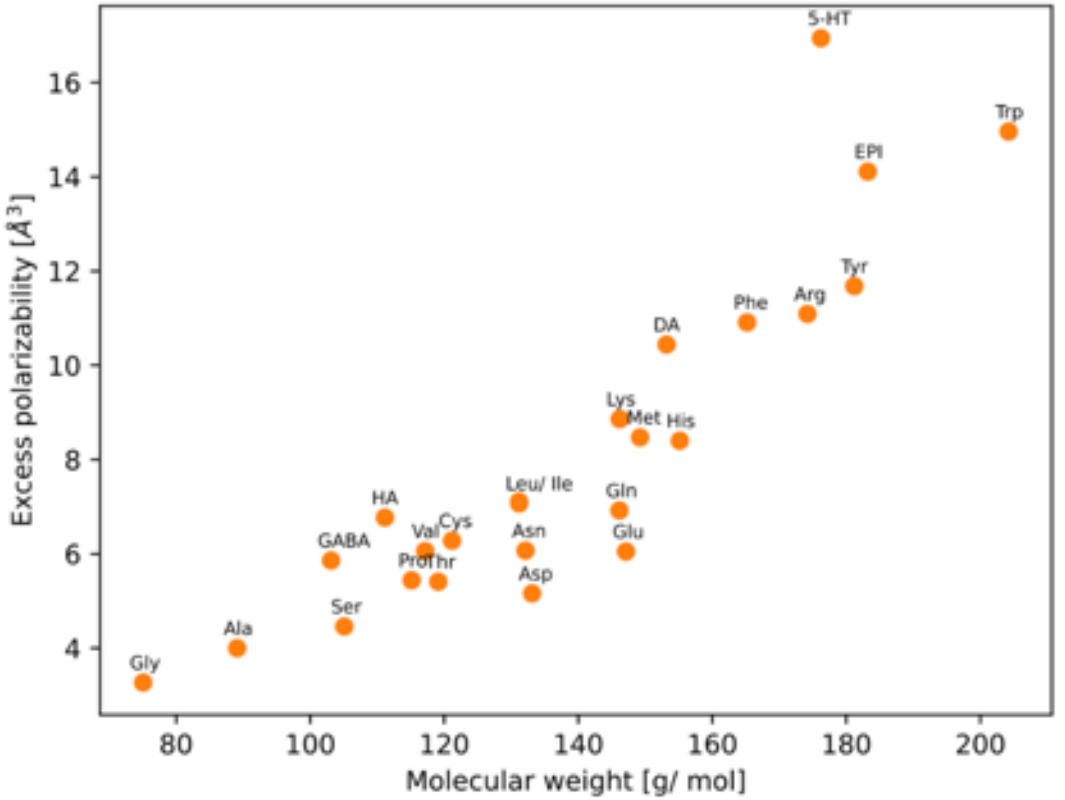
Laser wavelength

Effective volume of whispering gallery mode (from classical electromagnetism simulations)

Excess polarizability

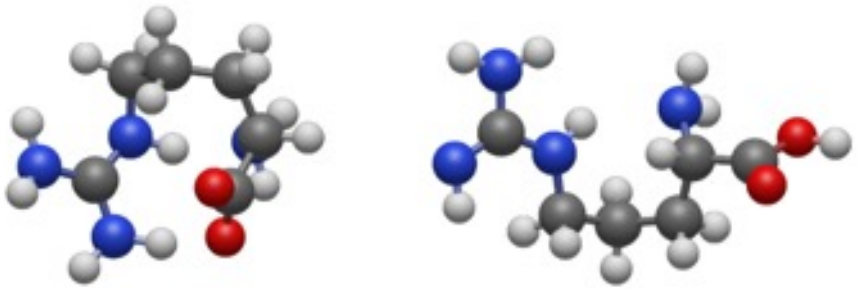
What is the effect of charge/ protonation state?

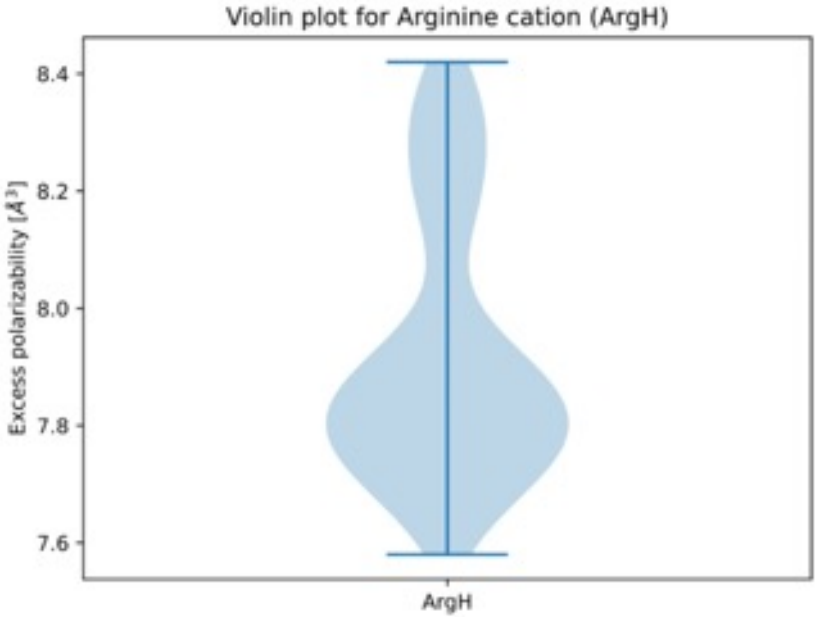




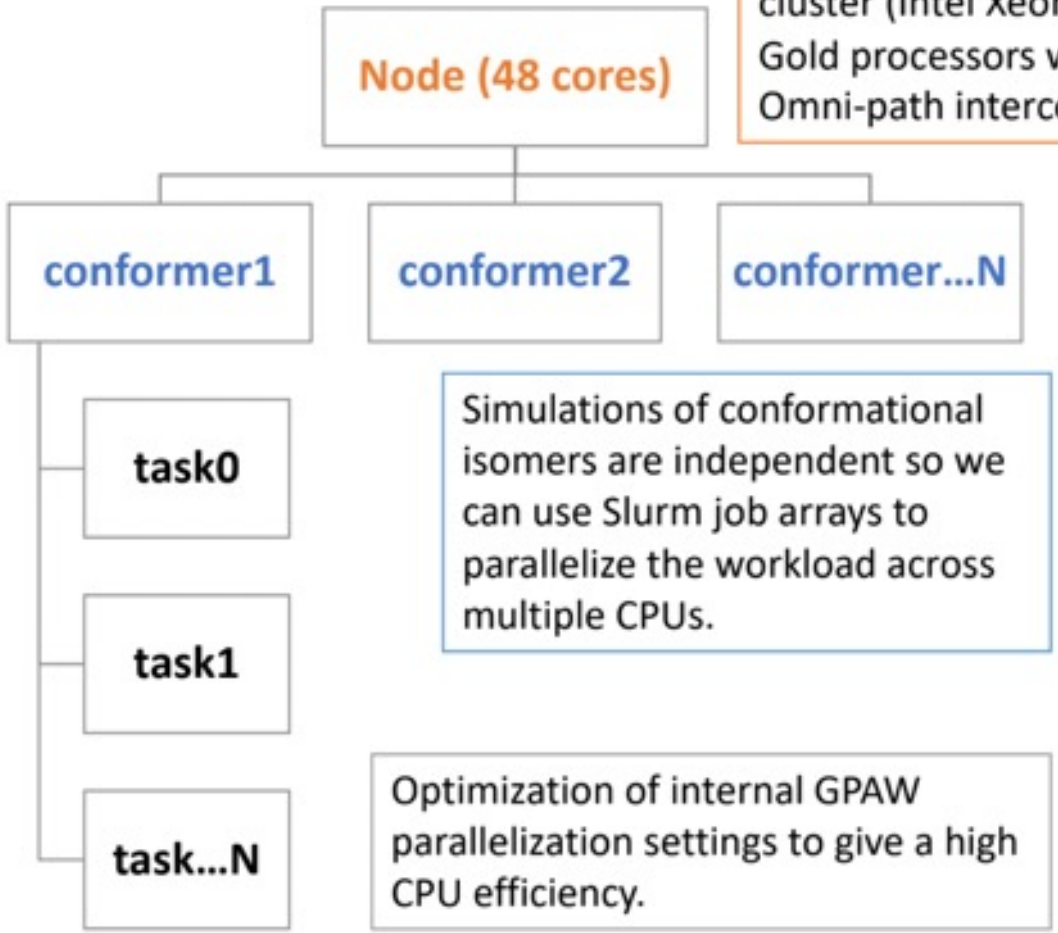
Excess polarizability

What about conformational isomers?





Running hundreds of jobs in parallel on the Justus2 cluster (Intel Xeon 6252 Gold processors with Omni-path interconnect).



Simulations of conformational isomers are independent so we can use Slurm job arrays to parallelize the workload across multiple CPUs.

Optimization of internal GPAW parallelization settings to give a high CPU efficiency.

Conclusions and outlook

Progress

- Decoding the biosensor signals by calculating the static polarizability of molecules and also by quantifying the statistical dispersion due to charge or conformational isomers.
- Using HPC resources to run hundreds of jobs in parallel, reducing the simulation time from several days to less than 1 hour.

Challenges

- It is not possible to use this method for optically active molecules. This requires a full time-dependent electronic structure calculation which is significantly more computationally intensive.

The authors acknowledge support by the state of Baden-Württemberg through bwHPC and the German Research Foundation (DFG) through grant no INST 40/575-1 FUGG (JUSTUS 2 cluster).

Ekaterina Zossimova
ez216@exeter.ac.uk

INTEGRATION OF A PARALLEL EFFICIENCY MONITORING TOOL INTO AN HPC PRODUCTION SYSTEM

Co-director, David Vicente	Co-director, Marta García-Gasulla	Ponent, Víctor López

Author, Helena Vela Beltran

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

UPC FIB

ISC

May 2023

CONTEXT

User Support Team

Best Practices for Performance and Programmability (BePPP)

Problem 01

HPC resources are not used properly.

Problem 02

Many scientific application developers do not come from a Computer Science background.

Problem 03

Performance analysis applications can be confusing and difficult to use for non-experienced users.

Problem 04

HPC users might not be aware of performance degradation.

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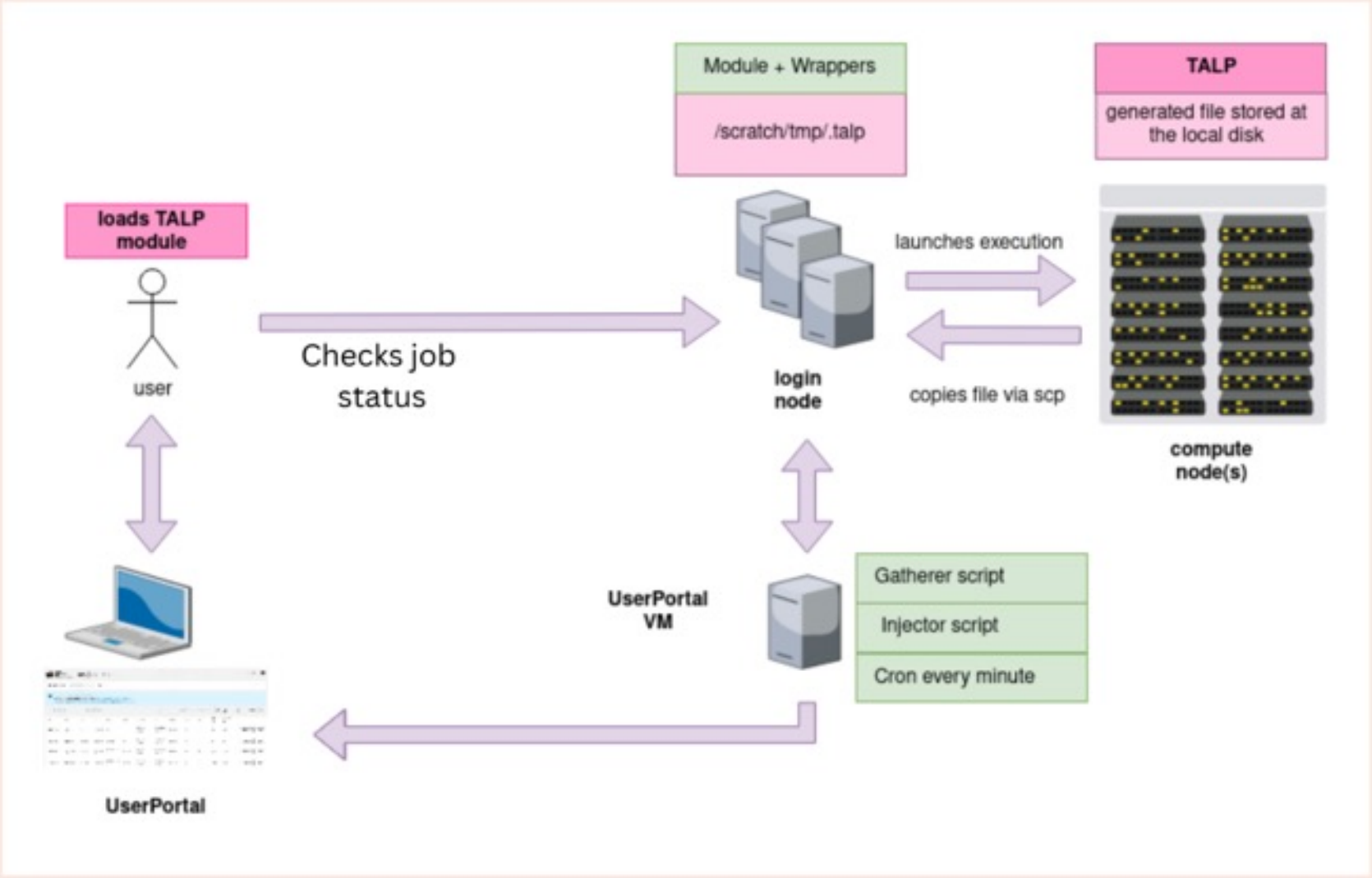
INTEGRATION SCHEMA



Results

TALP report

MPI Execution: MPI Execution
Elapsed Time: 0.00 s
Parallel Efficiency: 0.84
↳**Communication Efficiency:** 1.00
↳**Load Balance:** 0.84
↳ **lbIn:** 0.99
↳ **lbOut:** 0.85

THANK YOU!

Poster Reception

May 23, 2023

Foyer D-G

3:30 - 5:30 PM

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