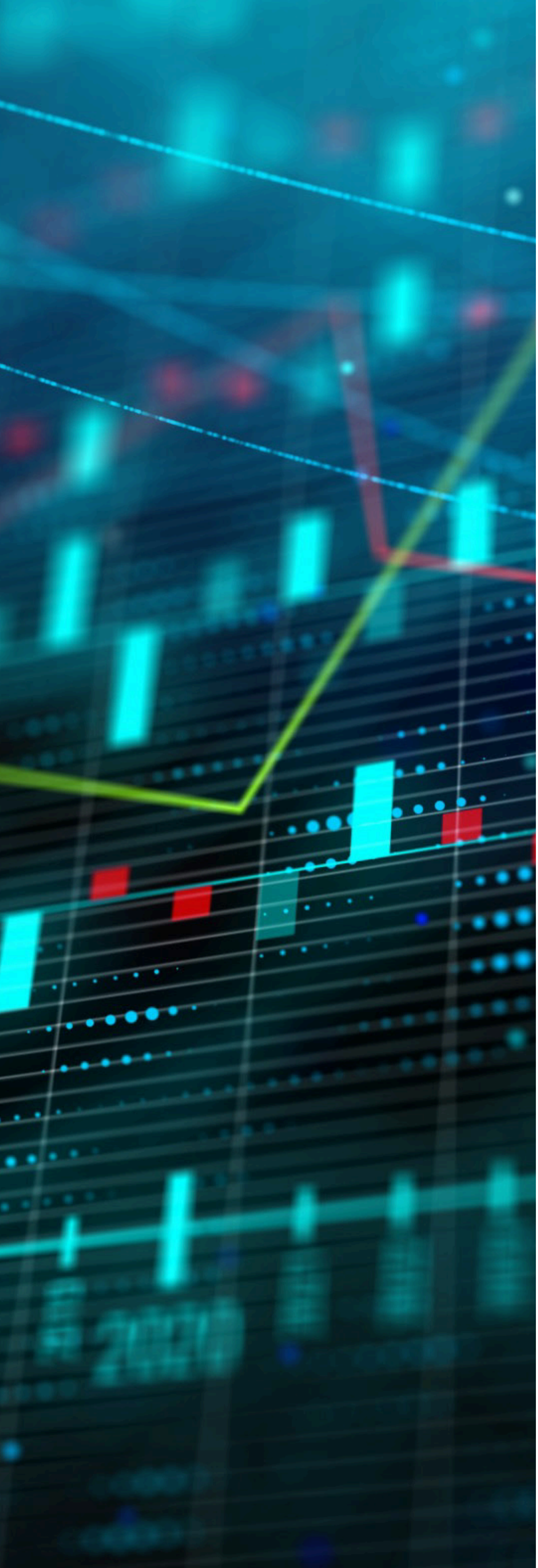


CONFERENCE PROGRAM

11TH EGU GALILEO CONFERENCE

Solid Earth and Geohazards in the Exascale Era

23 - 26 MAY 2023

BARCELONA (SPAIN)

Solid Earth and Geohazards in the Exascale Era

The geoscience community is multidisciplinary and transversal, encompassing Earth observatories, research and academia, model developers and, finally, model end-users and social agents. From a scientific point of view, the entire community is facing scientific breakthrough problems for which researchers need to share their knowledge and experience and make roadmap recommendations in order to contribute to the advancement of this rapidly growing field.

The 11th EGU Galileo Conference, titled *Solid Earth and Geohazards in the Exascale Era*, will bring together some of the world's best minds in various branches of computational geosciences to jointly tackle challenges and issues of Exascale computing.

This conference has been financially supported by the European Geosciences Union (EGU), the EuroHPC Center of Excellence for Exascale in Solid Earth (ChEESE) under Grant Agreement No 101093038 (https://cheese2.eu), the Ministry of Science and Innovation of Spain, the State Research Agency, and the European Union's Next Generation/PRTR Program through grant PCI2022-134973-2.

Table of Contents

Galileo Conferences

EGU Galileo Conferences are named in honor of Galileo Galilei, the famous Italian physicist, philosopher, astronomer and mathematician, universally recognized as the founder of modern science. The EGU Galileo Conferences address well-focused cutting-edge topics at the frontier of geosciences research. A limited number, typically about one hundred, internationally recognized scientists meet for 3 to 5 days to discuss and debate issues at the forefront of the discipline.

PAST MEETINGS

10th EGU Galileo Conference: The warm Pliocene: Bridging the geological data and modelling communities · Leeds, UK · 23–26 August 2022

7th EGU Galileo Conference: Second workshop on isotope-based studies of water partitioning and plant-soil interactions · Tuscany region, Italy · 26–28 July 2022

9th EGU Galileo Conference: Fire impacts at the Earth surface across space and time: perspectives for future fire management · Bad Belzig, Germany · 28 March – 1 April 2022

6th EGU Galileo Conference: Perturbations of earth surface dynamics caused by extreme events · Kathmandu, Nepal · 13–19 October 2019

5th EGU Galileo Conference: Mass extinctions, recovery and resilience · Utrecht, The Netherlands · 26 August – 1 September 2019

3rd EGU Galileo Conference: The anatomy of abrupt climate change: dissecting the palaeo-record to trace the mechanisms of climate variability · Gniew, Poland · 27–31 August 2018

4th EGU Galileo Conference: Exploring new frontiers in fluids processes in subduction zones · Leibnitz, Austria · 24–29 June 2018

2nd EGU Galileo Conference: Geoscience for understanding habitability in the solar system and beyond · São Miguel (Azores), Portugal · 25–29 September 2017

1st EGU Galileo Conference: From process to signal – advancing environmental seismology · Ohlstadt, Germany · 6–9 June 2017

Welcome Message

Prof. Arnau Folch · GEO3BCN - CSIC

Dear participants,

On behalf of the Organizing and Scientific Committees, it is my great pleasure to warmly welcome you to the 11th European Geosciences Union (EGU) Galileo Conference on Solid Earth and Geohazards in the Exascale Era.

As you may know, the underpinning concept of the Galileo Conferences is to gather a limited number of scientists working on cutting-edge topics, favoring informal discussions and debates on forefront scientific issues. In this edition, we want to tackle some of the challenges and opportunities that Exascale computing poses on (and offers to) geosciences.

The Conference is articulated around 4 sessions linked to corresponding trending topics, preparation and optimization of codes, edge-to-end data workflows, state-of-the-art in computational geosciences, and research infrastructures and access policies. In addition, the program also includes a series of aligned master classes to train and mentor early-career scientists. We explicitly invite you, participant of the Conference, to be proactive and participative during the breakout sessions, which should serve to write a consensual document defining the roadmap vision of our Community towards the Exascale era. In addition, we also encourage you to submit your contribution(s) to a special conference issue on Advances in Geosciences (ADGEO).

We want to express our gratitude to the EGU for supporting this event with organizational and financial support, which includes stipends to 10 Early Career Scientists prioritizing COST countries, and acknowledge the endorsement of the Center of Excellence for Exascale in Solid Earth (ChEESE).

Finally, I want to explicitly recognize the fantastic work that the Organizing Committee members (Rose Gregorio, Varvara Vedia, and María José García) have done over the last months in order to achieve an excellent and unforgettable event.

We hope that you will enjoy the Conference!

Prof. Arnau Folch

Committees

ORGANIZING COMMITTEE

Arnau Folch (GEO3BCN-CSIC)

Rose Gregorio (BSC - CNS)

Varvara Vedia (GEO3BCN-CSIC)

María José García (GEO3BCN-CSIC)

MASTER CLASS INSTRUCTORS

Ludovic Raess (ETH Zurich)

Ivan Utkin (ETH Zurich)

Rosa M. Badia (BSC - CNS)

Javier Conejero (BSC - CNS)

Raül Sirvent (BSC - CNS)

Daniele Lezzi (BSC - CNS)

Jorge Macías (University of Malaga)

Rui Ferreira (CERIS - University of Lisbon)

Arnau Folch (GEO3BCN-CSIC)

Nicola Castelletto (LLNL)

SCIENTIFIC COMMITTEE

Arnau Folch (GEO3BCN-CSIC)

Josep de la Puente (BSC - CNS)

Rui Ferreira (CERIS - University of Lisbon)

Alice-Agnes Gabriel (LMU Munich)

Boris Kaus (JGU Mainz)

Laetitia Le Pourhiet (Sorbonne Université Paris)

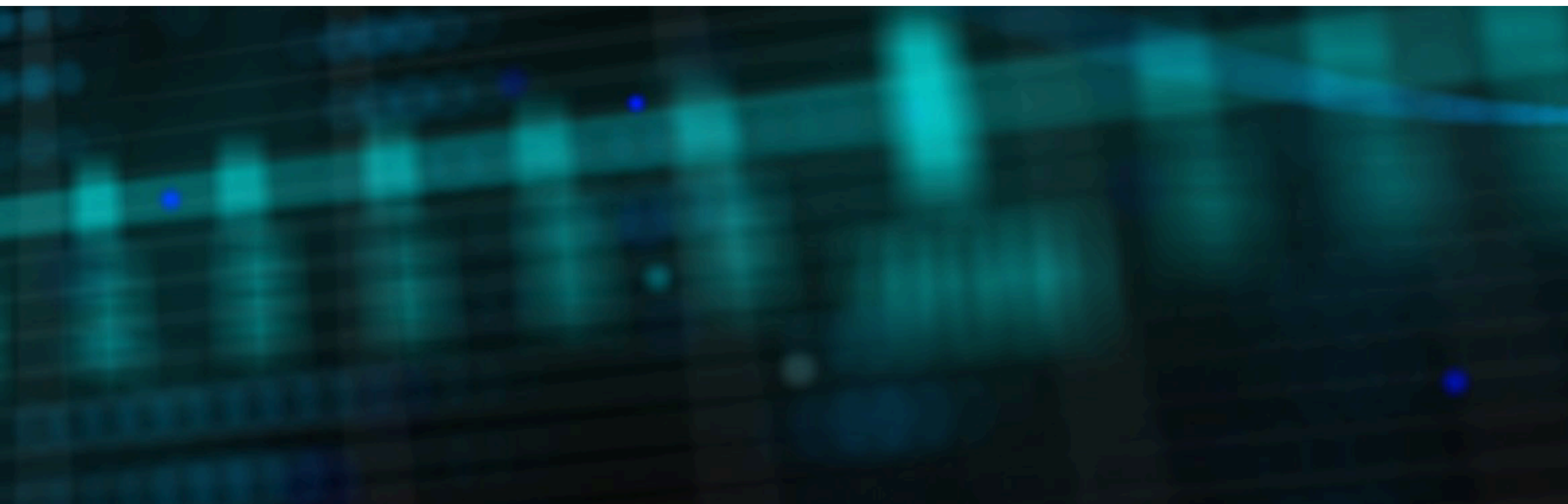
Jorge Macias (University of Malaga)

Marta Pienkowska (ETH Zurich)

Tiziana Rossetto (University College London)

Victor Vilarrasa (IDAEA - CSIC)

Marisol Monterrubio (BSC - CNS)



Keynote Speakers

SESSION 1 · Wednesday 24 April 2023

Preparation and optimization of HPC codes to Exascale

Richard Tran Mills

Enabling End-to-End Accelerated Multiphysics Simulations in the Exascale Era Using PETSc

SESSION 2 · Wednesday 24 April 2023

Edge-to-end data workflows

Scott Callaghan

Preparing Seismic Applications for Exascale Using Scientific Workflows

SESSION 3 · Thursday 25 April 2023

State-of-the-art in computational geosciences

Nicola Castelletto

Simulation of Geological CO2 Storage with the GEOS Open-Source Multiphysics Simulator

SESSION 4 · Thursday 25 April 2023

Horizon Europe and EuroHPC Policies

Linda Gesenhues

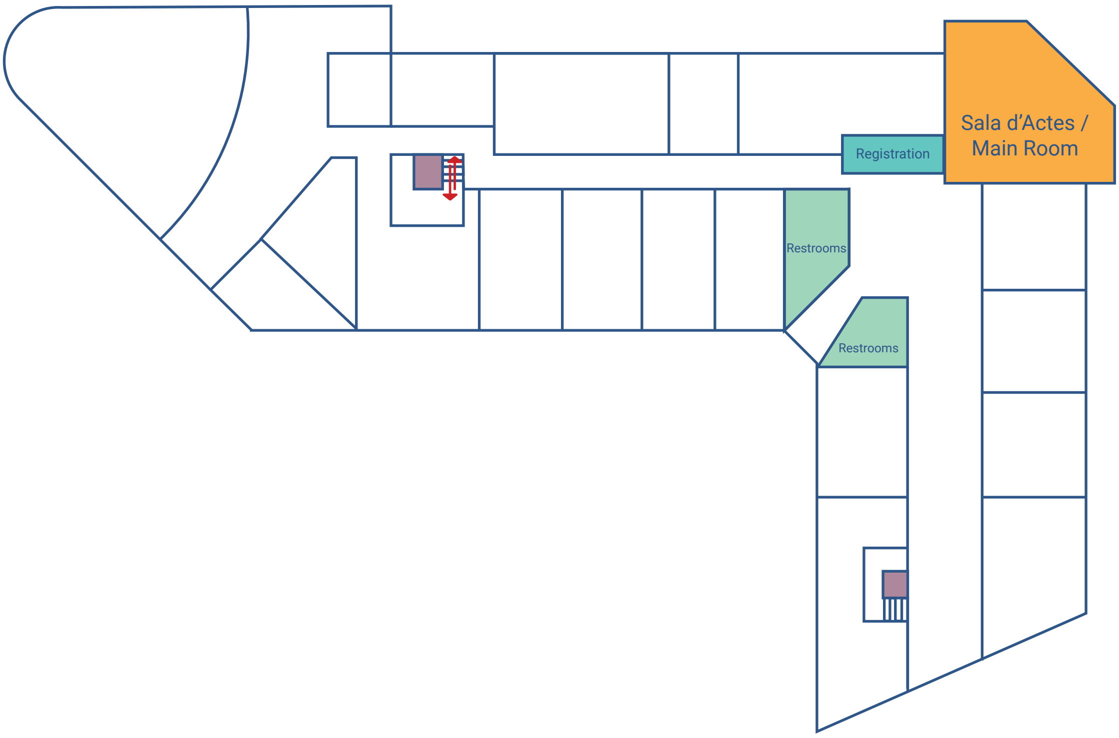
The European High Performance Computing Joint Undertaking (EuroHPC JU) – Leading the way in European Supercomputing

Venue Map

The classes and conferences of the 11th EGU Galileo Conference will mainly take place on the Vèrtex building on the North Campus of the Polytechnic University of Catalonia (UPC).

Address: Vèrtex Building (VX), Plaça d'Eusebi Güell, 6, 08034 Barcelona

BASEMENT LEVEL 1



BASEMENT LEVEL 2

Program

Master Classes · Tuesday 23 May 2023

	MASTER CLASS	INSTRUCTORS
1	**Preparation and optimization of HPC codes to Exascale**	Ludovic Raess (ETH Zurich) Ivan Utkin (ETH Zurich)
2	**Edge-to-end data workflows**	Rosa M. Badia (BSC) Javier Conejero (BSC) Raül Sirvent (BSC) Daniele Lezzi (BSC)
3	**State-of-the-art in computational geosciences**	Jorge Macías (University of Malaga) Rui Ferreira (CERIS-University of Lisbon) Arnau Folch (CSIC) Nicola Castelletto (LLNL)

TIME	MC1	MC2&3
9:00-11:00	• Introduction by Masters (GPU HPC) • Student short presentation (5 min) about themselves, their research interests and their vision of exascale supercomputing • Getting set-up with GPU node access on BSC computing system • Brief intro about Julia for HPC	• Introduction by Masters • Presentation by students (30 min each in total, including discussion and interaction)
11:00-11:30	*Coffee break (provided)* *VX S217*	
11:30-13:30	Hands-on I: • GPU computing for HPC	

TIME	MC1	MC2&3
11:30-13:30	• Julia GPU + MPI stack • Model design and implementation: Stokes flow in a channel	
13:30-14:30	*Lunch (not provided)* *Around UPC Campus*	
14:30-16:30	Hands-on II: • Multi-GPU computing • Performance measures (effective memory throughput)	• Master pitch presentation • Master Class Plenary Session (more collective discussion) • Lessons learnt
16:30-17:00	*Coffee break (provided)* *VX S217*	
17:00-19:00	**Option 1: Towards scalable inverse modeling** (Hands-on III): • AD tools in Julia • Computing the Jacobian-vector product (JVP) in our multi-GPU model • Advanced: adjoint solutions and optimisation problems • Wrap-up and collaborative discussion among students and masters	**Option 2. Hackathon:** This slot will focus on the development of workflows with PyCOMPSs. The session will target the aspects derived from the challenges and bottlenecks indicated by the students in their presentations. The hackathon will be very practical, describing first the challenge and possible solutions and then solving them in a real set-up in one of the BSC computing systems.
19:00-20:30	*Icebreaker event · Light dinner* *Vertex Garden*	

Session 1 · Wednesday 24 May 2023

Preparation and optimization of HPC codes to Exascale
Conveners: Boris Kaus and Marisol Monterrubio-Velasco

TIME	ROOM	SESSION 1
8:30-8:45	Sala d'Actes	Registration
8:45-9:00		Welcome, conference organization and short introduction of participants
9:00-10:00		Keynote · Richard Mills **Enabling End-to-End Accelerated Multiphysics Simulations in the Exascale Era Using PETSc**
10:00-10:15		Short talk · Marc de la Asuncion **Towards exascale-prepared codes for tsunami simulation**
10:15-10:30		Short talk · Ivan Utkin **Massively parallel inverse modelling on GPUs using the adjoint method**
10:30-11:30	VX S217	*Coffee break (provided)* *Poster session for Session 1* Albert de Montserrat Navarro **Using Julia for the next generation of HPC-ready software for geodynamic modelling** Daniel Caviedes-Voullième **Towards exascale shallow-water modelling with SERGHEI model and Kokkos** Pascal Aellig **Modelling the accumulation of magma prior to the caldera collapse** Kim Olsen **AWP-ODC: A Highly Scalable HPC Tool for Dynamic Rupture and Wave Propagation Simulations** Learn more at: https://youtu.be/VgOR2JEDZIg Casper Pranger **Tandem: A discontinuous Galerkin method for sequences of earthquakes and aseismic slip on multiple faults using unstructured curvilinear grids**

11:30-12:30	Sala d'Actes & VX S218	Breakout Sessions
12:30-13:00	Sala d'Actes	Plenary discusion
13:00-14:30	Around UPC Campus	*Lunch (not provided)*

Session 2 · Wednesday 24 May 2023

Edge-to-end data workflows
Conveners: Josep de la Puente, Rui Ferreira and Tiziana Rossetto

TIME	ROOM	SESSION 2
14:30-15:30	Sala d'Actes	Keynote · Scott Callaghan **Preparing Seismic Applications for Exascale Using Scientific Workflows**
15:30-15:45		Short talk · Natalia Poiata **BackTrackBB workflow for seismic source detection and location with PyCOMPSs parallel computational framework**
15:45-16:00		Short talk · Steve Gibbons **ML Emulation of High Resolution Inundation Maps for Probabilistic Tsunami Hazard Analysis**
16:00-16:15		Short talk · Antonio Costa **Improving Probabilistic Gas Hazard Assessment through HPC: Unveiling VIGIL-2.0, an automatic Python workflow for probabilistic gas dispersion modelling**
16:15-16:30		Short talk · Farnaz Bayat **A first look at the calibration of near-fault motion models to synthetic big data from CyberShake's application to the Southwest Iceland transform zone**
16:30-17:30	Sala d'Actes & VX S218	Breakout Sessions
17:30-18:00	Sala d'Actes	Plenary discusion

Session 2 · Wednesday 24 May 2023

Edge-to-end data workflows
Conveners: Josep de la Puente, Rui Ferreira and Tiziana Rossetto

TIME	ROOM	SESSION 2
18:00-19:00	VX S217	*Coffee break (provided)* *Poster session for Session 2* Sebastian Noe **The Collaborative Seismic Earth Model: Generation 2** Alejandra Guerrero **Volcanic ash dispersal and deposition workflow on HPC** Marisol Monterrubio-Velasco **Machine Learning based Estimator for ground Shaking maps** Learn more at: https://youtu.be/QrWXSHqx1wI Farnaz Bayat **A new Near-Fault Earthquake Ground Motion Model for Iceland from Bayesian Hierarchical Modeling** Milad Kowsari **Characterization of Earthquake Near-fault Ground Motion Parameters Using an Artificial Neural Network on Synthetic Big Data** Benedikt Halldorsson **Towards physics-based finite-fault Monte Carlo PSHA for Southwest Iceland based on a new fault system model** Luciano Garone **Monitoring the sediment dynamics of Maltese beaches. The SIPOBED project and its future challenges** Nishtha Srivastava **Real time Earthquake detection using Deep Learning**
20:00 - 22:00	Restaurante Pomarada	*Social Dinner*

Session 3 · Thursday 25 May 2023

State-of-the-art in computational geosciences
Conveners: Victor Vilarrasa and Jorge Macias

TIME	ROOM	SESSION 3
8:30-09:00	Sala d'Actes	Registration
9:00-10:00		Keynote · Nicola Castelleto **Simulation of Geological CO2 Storage with the GEOS Open-Source Multiphysics Simulator**
10:00-10:15		Short talk · Arnau Folch **HPC projects in the Solid Earth ecosystem**
10:15-10:30		Short talk · Louise Cordrie **Complete workflow for tsunami simulation and hazard calculation in urgent computing using HPC services**
10:30-11:00	VX S217	*Coffee break (provided)*
11:00-11:15	Sala d'Actes	Short talk · Carlos Paredes **Can we model lava flows faster than real-time to assist on a first volcanic emergency response?**
11:15-11:30		Short talk · Iva Tojčić **Modelling of extreme sea-level hazards: state-of-the-art and future challenges**
11:30-12:30	Sala d'Actes & VX S218	Breakout Sessions
12:30-13:00	Sala d'Actes	Plenary discusion
13:00-14:30	Around UPC Campus	*Lunch (not provided)*

Session 4 + Session 3 · Thursday 25 May 2023

Horizon Europe and EuroHPC Policies
Conveners: Arnau Folch and Laetitia Le Pourhiet

TIME	ROOM	SESSION 4
14:30-15:00	Sala d'Actes	Keynote · Linda Gesenhues **The European High Performance Computing Joint Undertaking (EuroHPC JU) – Leading the way in European Supercomputing**
15:00-15:15	Sala d'Actes	Invited Talk · Oriol Pineda **Access to MareNostrum5 and other European HPC infrastructures**
15:15-15:30	Sala d'Actes	Invited Talk · Thomas Zwinger **LUMI supercomputer for European researchers**
15:30-15:45	Sala d'Actes	Invited Talk · Piero Lanucara **Leonardo: A Simulator4Earth**
15:45-16:00	Sala d'Actes	Invited Talk · Ignacio Sarasua **Accelerating Time-To-Science in Geophysical Simulations**
16:00-16:30	Sala d'Actes & VX S218	Breakout session
16:30-17:00	Sala d'Actes	Plenary discusion
TIME	**ROOM**	**SESSION 3**
17:00-18:00	VX S217	*Coffee break (provided)* *Poster session for Session 3* Tomaso Esposti Ongaro **Three-dimensional, multiphase flow numerical models of phreatic volcanic eruptions** Auregan Boyet **Hydro-mechanical modeling of injection-induced seismicity at the Deep Heat Mining Project of Basel, Switzerland**

Session 3 · Thursday 25 May 2023

State-of-the-art in computational geosciences
Conveners: Victor Vilarrasa and Jorge Macìas

TIME	ROOM	SESSION 3
17:00-18:00	VX S217	Iman R. Kivi **A computationally efficient numerical model to understand potential CO2 leakage risk within gigatonne scale geologic storage** Cláudia Reis **Tsunami risk management in the Exascale Era:Global advances and the European standpoint** Juan Francisco Rodríguez Gálvez **Combining High-Performance Computing and Neural Networks for Tsunami Maximum Height and Arrival Time Forecasts** Manuel Stocchi **Ash fallout long term probabilistic volcanic hazard assessment for Neapolitan volcanoes: an example of what Earth Scientists can do with HPC resources** Learn more at: https://youtu.be/xVEfrt8bCQM Deepak Garg **GALES: a general-purpose multi-physics FEM code** Carlos Sánchez-Linares **HPC in Rapid Disaster Response: Numerical simulations for hazard assessment of a potential dam breach of the Kyiv cistern reservoir, Ukraine** Learn more at: https://youtu.be/bA2stMHCZX4 Linus Walter **Physics-informed Neural Networks to Simulate Subsurface Fluid Flow in Fractured Media** Thomas Zwinger **Coupled permafrost-groundwater simulation applied to a spent fuel nuclear waste repository** Learn more at: https://youtu.be/zg0iNVN4T3Y Haiqing Wu **Risk assessment and mitigation of induced seismicity for geo-energy related applications at the basin scale** Alice Abbate **Optimal source selection for local probabilistic tsunami hazard analysis** Alejandro Gonzalez del Pino **Exhaustive High-Performance Computing utilization in the estimation of the economic impact of tsunamis on Spanish coastlines** Victor Vilarrasa **Numerical simulation of injection-induced seismicity**

Session 3 · Thursday 25 May 2023

State-of-the-art in computational geosciences
Conveners: Victor Vilarrasa and Jorge Macías

TIME	ROOM	SESSION 3
17:00-18:00	VX S217	Natalia Zamora **Tsunami evacuation using an agent-based model in Chile** Leonardo Mingari **A digital twin component for volcanic dispersal and fallout** Andrea C. Riaño **Integrating 3D physics-based earthquake simulations to seismic risk assessment: The case of Bogotá, Colombia** Ebissa Kedir **Modeling Depth averaged velocity and Boundary Shear Stress distribution with complex flows** Learn more at: https://youtu.be/iIPfXj5boBY
18:00-19:00	BSC building & Torre Girona Chapel	Visit to MareNostrum 4 and 5 supercomputers

Session 4 · Friday 26 May

TIME	ROOM	
9:00-10:30	Sala d'Actes	Discussion on the the consensual documents
10:30-11:00	VX S217	*Coffee break (provided)*
11:00-12:00	Sala d'Actes	Further discussion on the the consensual documents
12:00-12:30	Sala d'Actes	Wrap up

List of Participants

Alice Abbate (University of Trieste)

Claudia Abril (BSC-CNS)

Pascal Aellig (Johannes Gutenberg-University Mainz)

Rosa M. Badia (BSC-CNS)

Farnaz Bayat (University of Iceland)

Mathis Bergogne (Sorbonne Université)

Cedric Bhihe (BSC-CNS)

Rut Blanco Prieto (BSC-CNS)

Auregan Boyet (GEO3BCN-CSIC)

Eduardo César Cabrera Flores (BSC-CNS)

Scott Callaghan (University of Southern California)

Ramon Carbonell (GEO3BCN-CSIC)

Nicola Castelletto (Lawrence Livermore National Laboratory)

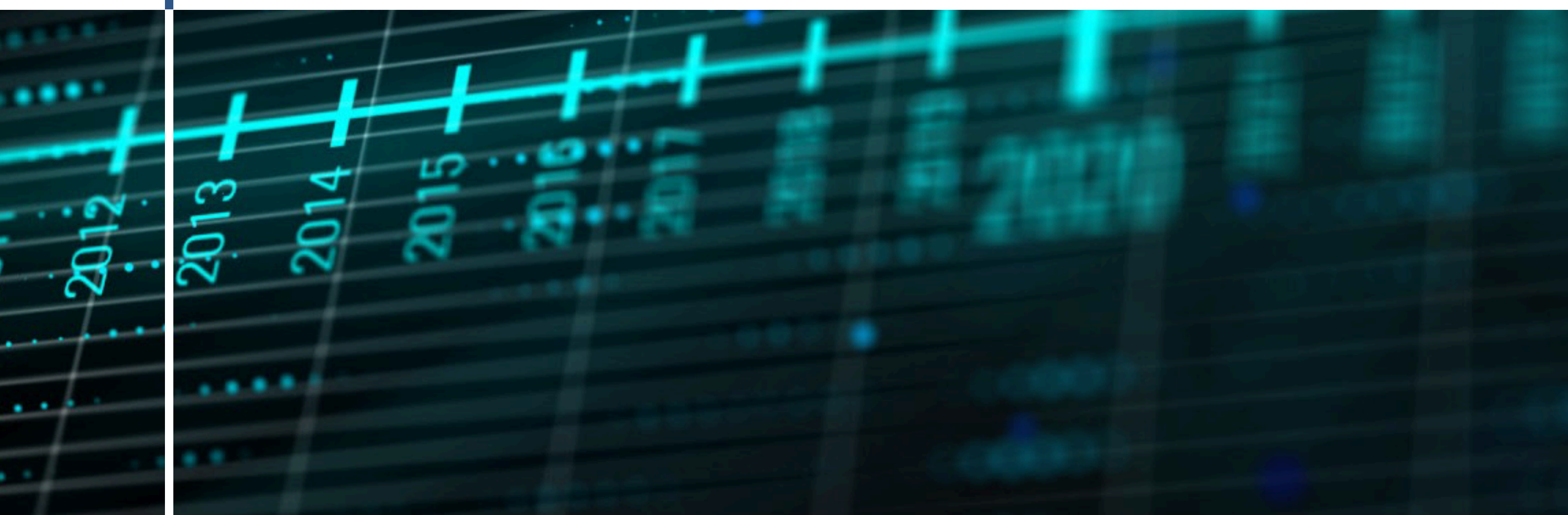
Octavio Castillo Reyes (BSC-CNS)

Daniel Caviedes-Voullième (Forschungszentrum Jülich)

Louise Cordrie (INGV)

Antonio Costa (INGV)

Marc de la Asunción (Universidad de Málaga)



Josep de la Puente (BSC-CNS)

Albert de Montserrat Navarro (ETH Zurich)

Tomaso Esposti Ongaro (INGV)

Rui Miguel Ferreira (Instituto Superior Tecnico, Universidade de Lisboa)

Arnau Folch (GEO3BCN-CSIC)

Ebissa Gadissa (Debre Tabor University)

Luciano Galone (University of Malta)

María Jose García Miraz (GEO3BCN-CSIC)

Deepak Garg (INGV)

Linda Gesenhues (EuroHPC JU)

Steven Gibbons (NGI)

Flora Giudicepietro (INGV)

Alex Gonzalez del Pino (Universidad de Málaga)

Rose Gregorio (BSC-CNS)

Alejandra Guerrero (GEO3BCN-CSIC)

Benedikt Halldórsson (University of Iceland / Icelandic Meteorological Office)

Paula Herrero-Barbero (GEO3BCN-CSIC)

Camille Huynh (CNRS ITES UMR7063 / Febus Optics)

Boris Kaus (Johannes-Gutenberg University Mainz)

Milad Kowsari (University of Iceland)

Piero Lanucara (CINECA)

Laetitia Le Pourhiet (Sorbonne Université)

Daniele Lezzi (BSC-CNS)

Giovanni Macedonio (Istituto Nazionale di Geofisica e Vulcanologia)

Jorge Macias (University of Malaga)

Marc Martínez Sepúlveda (GEO3BCN-CSIC)

Richard Tran Mills (Argonne National Laboratory)

Leonardo Mingari (GEO3BCN-CSIC)

Marisol Monterrubio-Velasco (BSC-CNS)

Sebastian Noe (ETH Zurich)

Kim Olsen (San Diego State University)

Carlos Paredes Bartolome (Politécnica de Madrid)

Jordi Petchamé

Oriol Pineda (BSC - CNS)

Natalia Poiata (National Institute for Earth Physics)

Casper Pranger (LMU Munich)

Iman Rahimzadeh Kivi (IDAEA)

Cláudia Reis (IST Lisbon University)

Andrea Riaño Escandon (Universidad de los Andes)

Joachim Rimpot (University of Strasbourg)

Juan Francisco Rodríguez Gálvez (University of Málaga)

Tiziana Rossetto (University College London)

Ludovic Räss (ETH Zurich)

Ignacio Sarasua (NVIDIA)

Chiara Scaini (National Institute of Oceanography and Applied Geophysics)

Felix-Marian Skwarczynski (SLB)

Carlos Spa (BSC-CNS)

Nishtha Srivastava (Frankfurt Institute for Advanced Studies)

Manuel Stocchi (Università degli Studi Aldo Moro di Bari)

Carlos Sánchez-Linares (University of Málaga)

Hui Ang (Helmholtz-Zentrum Potsdam Deutsches GeoForschungsZentrum GFZ)

Iva Tojcic (Ruder Boškovic Institute)

Ivan Utkin (ETH Zürich)

Varvara Vedia (GEO3BCN-CSIC)

Rubén Vidal (Universitat Politècnica de Catalunya)

Victor Vilarrasa (IDAEA - CSIC)

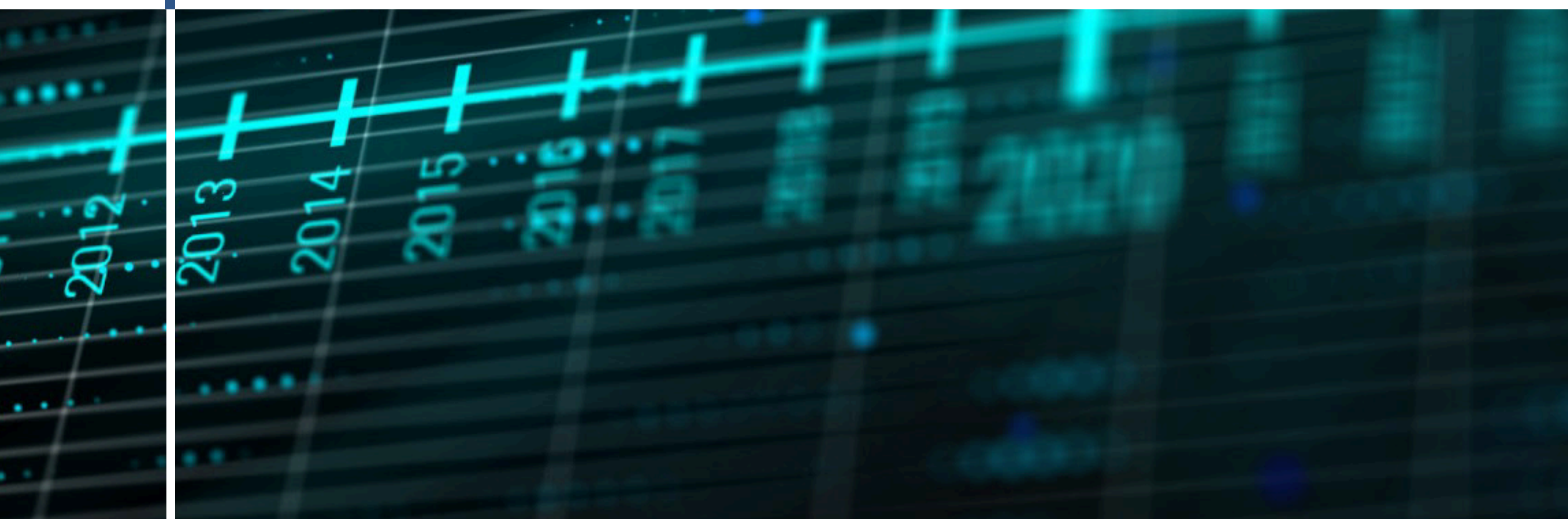
Linus Walter (CSIC)

Natalia Zamora (BSC-CNS)

Zhao Zixiong (Zhejiang University)

Thomas Zwinger (CSC - IT Center for Science Ltd.)

Abstracts



SESSION 1 PREPARATION AND OPTIMIZATION OF HPC CODES TO EXASCALE

KEYNOTE SPEAKER

Enabling End-to-End Accelerated Multiphysics Simulations in the Exascale Era Using PETSc

Richard Tran Mills[1], Mark Adams[2], Satish Balay[1], Jed Brown[3], Jacob Faibussowitsch[1], Matthew G. Knepley[4], Scott Kruger[5], Hannah Morgan[6], Todd Munson[1], Karl Rupp[7], Barry Smith[8], Stefano Zampini[9], Hong Zhang[1], and Junchao Zhang[1]

[1]Argonne National Laboratory · [2]Lawrence Berkeley National Laboratory · [3]University of Colorado Boulder
[4]University at Buffalo · [5]Tech-X Corporation · [6]University of Chicago · [7]Technische Universität Wien
[8]Flatiron Institute· [9]King Abdullah University of Science & Technology (KAUST)

The Portable Extensible Toolkit for Scientific Computation (PETSc) library provides scalable solvers for nonlinear time-dependent differential and algebraic equations and for numerical optimization; it is used in dozens of scientific fields, and has been an important building block for many computational geoscience applications. Starting from the terascale era in the 1990s and continuing into the present dawn of the exascale era, a major goal of PETSc development has been achieving the scalability required to fully utilize leadership-class supercomputers. We will describe some of the algorithmic developments made during the era in which achieving inter-node scalability was the primary challenge to enabling extreme-scale computation, and then survey the challenges posed by the current era in which harnessing the abundant fine-scale parallelism within compute nodes -- primarily in the form of GPU-based accelerators -- has assumed at least equal importance.

We will discuss how the PETSc design for performance portability addresses these challenges while stressing flexibility and extensibility by separating the programming model used by application code from that used by the library. Additionally, we will discuss recent developments in PETSc's communication module, PetscSF, that enable flexibility and scalable performance across large GPU-based systems while overcoming some of the difficulties posed by working directly with the Message Passing Interface (MPI) on such systems. A particular goal of this talk will be to go beyond simply describing the work performed to prepare PETSc and simulation codes that rely on it to run on exascale-class systems, but to enumerate the challenges we encountered and to share the essential lessons learned that can help other developers to prepare and optimize their high-performance scientific computing codes for the exascale era.

SHORT TALKS

Towards exascale-prepared codes for tsunami simulation

Marc de la Asunción, Jorge Macías, and Manuel Jesús Castro

Universidad de Málaga, Dpto. Análisis Matemático, Estadística e Investigación Operativa, y Matemática Aplicada, Málaga, Spain

The recently finished ChEESE European project aimed at establishing a center of excellence in the domain of solid earth by developing ten flagship European codes prepared for the upcoming exascale supercomputers. The EDANYA group, at the University of Malaga, Spain, has developed two of these flagship codes: Tsunami-HySEA and Landslide-HySEA, for the simulation of tsunamis generated by earthquakes and landslides, respectively. These two codes, although being already implemented for multi-gpu architectures at the beginning of the ChEESE project, underwent substantial changes during the lifetime of the project with the objective of improving several crucial aspects such as their efficiency, scaling or input/output requirements. Specifically, we added features such as an improved load balancing, direct GPU to GPU data transfers or compressed output files, among others. Additionally, we developed a version of Tsunami-HySEA, named Monte-Carlo, particularly suited for areas such as probabilistic tsunami forecast or machine learning, capable of performing multiple simulations in parallel. In this presentation we describe all these developments carried out during the ChEESE project, along with the two audits that the two codes went through, performed by the Performance Optimisation and Productivity Centre of Excellence in HPC (POP CoE). Finally, we show some comparative results using realistic scenarios achieved at the beginning and at the end of the project.

Massively parallel inverse modelling on GPUs using the adjoint method

Ivan Utkin[1,2] and Ludovic Räss[1,2]

[1]Laboratory of Hydraulics, Hydrology and Glaciology (VAW), ETH Zurich, Zurich, Switzerland, [2]Swiss Federal Institute for Forest, Snow and Landscape Research (WSL), Birmensdorf, Switzerland

Continuum-based numerical modelling is a useful tool for interpreting field observations and geological or geotechical data. In order to match the available data and the results of numerical simulations, it is necessary to estimate the sensitivity of a particular model to changes in its parameters. Recent advances in hardware design, such as the development of massively parallel graphical processing units (GPUs), make it possible to run simulations at unprecedented resolution close to that of the original data. Thus, automated methods of calculating the sensitivity in a high-dimensional space of parameters are in demand.

The adjoint method of computing sensitivities, i.e., gradients of the forward model solution with respect to the parameters of interest, gains more attention in the scientific and engineering communities. This method allows for computing the sensitivities for every point of computational domain using the results of only one forward solve, in contrast to the direct method that would require runninng the forward simulation for each point of the domain. This property of adjoint method significantly reduces the amount of computational resources required for sensitivity analysis and inverse modelling.

In this work, we demonstrate the applications of the adjoint method to inverse modelling in geosciences. We developed massively parallel 3D forward and inverse solvers with full GPU support using Julia language. We present the results of performance and scalability tests on Piz Daint supercomputer at CSCS.

POSTERS

Using Julia for the next generation of HPC-ready software for geodynamic modelling

Albert de Montserrat Navarro[1], Boris Kaus[2], Ludovic Räss[3], Ivan Utkin[3], and Paul Tackley[1]

[1]Institute of Geophysics (ERDW), ETH Zürich, Switzerland, [2]Institute of Geosciences, Johannes-Gutenberg University Mainz, Germany, [3]Laboratory of Hydraulics, Hydrology and Glaciology (VAW), ETH Zürich, Switzerland

Following the long-standing paradigm in HPC, scientific software has been typically written in high-level statically typed and compiled languages, namely C/C++ and Fortran. The arguably low productivity rates of these languages led to the so-called two-language problem, where dynamic languages such as Python or MATLAB are used for prototyping purposes, before porting the algorithms to high-performance languages. The Julia programming language aims at bridging the productivity rates and other advantages of such dynamic languages without sacrificing the performance provided by their static counterparts. The combination of this high performance, productivity rates and other powerful tools, such as advanced meta-programming (i.e. code generation), make Julia a suitable candidate for the next generation of HPC-ready scientific software.

We introduce the open-source and Julia-written package JustRelax.jl (https://github.com/PTsolvers/JustRelax.jl) as a way forward for the next generation of geodynamic codes. JustRelax.jl is a production-ready API for

for a collection of highly-efficient numerical solvers (Stokes, diffusion, etc.) based on the embarrassingly parallel pseudo-transient method. We rely on ParallelStencil.jl (https://github.com/omlins/ParallelStencil.jl), which leverages the advanced meta-programming capabilities of Julia to generate efficient computational kernels agnostic to the back-end system (i.e. Central Processing Unit (CPU) or Graphics Processing Unit (GPU)). Using ImplicitGlobalGrid.jl (https://github.com/eth-cscs/ImplicitGlobalGrid.jl) to handle the MPI and CUDA-aware MPI communication, these computational kernels run seamlessly in local shared-memory workstations and distributed memory and multi-GPU HPC systems with little effort for the front-end user.

Efficient computation of the (local) physical properties of different materials is another critical feature required in geodynamic codes, for which we employ GeoParams.jl (https://github.com/JuliaGeodynamics/GeoParams.jl). This package provides lightweight, optimised, and reproducible computation of different material properties (e.g. advanced rheological laws, density, seismic velocity, etc.), amongst other available features. GeoParams.jl is also carefully designed to support CPU and GPU devices, and be fully compatible with other external packages, such as ParallelStencil.jl and existing auto-differentiation packages.

We finally show high-resolution GPU examples of geodynamic models based on the presented open-source Julia tools.

Towards exascale shallow-water modelling with SERGHEI model and Kokkos

Daniel Caviedes-Voullième[1], Mario Morales-Hernández[2], and Ilhan Özgen-Xian[3]

[1]SimDataLab Terrestrial Systems, Forschungszentrum Jülich, Jülich, Germany, [2]Fluid Mechanics, I3A-University of Zaragoza, Zaragoza, Spain, [3]Institute of Geoecology, Technische Universität Braunschweig, Braunschweig, Germany

The Simulation EnviRonment for Geomorphology, Hydrodynamics and Ecohydrology in Integrated form (SERGHEI) model framework is a model framework for environmental hydrodynamics, ecohydrology, morphodynamics, and, importantly, interactions and feedbacks among such processes. SERGHEI is designed to be applicable to both geoscientific questions of coupled processes in Earth system science such as hydrological connectivity and river stability, as well as engineering applications to flooding and transport phenomena.

In this contribution we present the SERGHEI model framework, its modular concept and its performance-portable implementation. We discuss the implementation of SERGHEI including the specifics of a highly efficient parallel implementation of the numerical scheme (based on augmented Riemann solvers) and how we achieve portability using the Kokkos programming model as an abstraction layer. The experience in SERGHEI suggests that Kokkos is a robust path towards performance-portability, and sets a realistic path for SERGHEI to be ready for the upcoming European exascale systems.

We focus on the SERGHEI-SWE module which solves 2D shallow-water equation. We show that this fully operational module is performance-portable across CPUs and GPUs in several TOP500 systems, as well as first results on portability across GPU vendors. We discuss the computational performance on benchmark problems and show its scalability into the range of hundreds of scientific-grade GPUs. Additionally, we show first results of performance of the upcoming transport module in SERGHEI, and discuss the computational implications and outlook considering further integration of new modules and solvers in SERGHEI.

Modelling the accumulation of magma prior to the caldera collapse

Pascal Aellig[1], Boris Kaus[1], Albert de Montserrat[2], Daniel Kiss[1], and Nicolas Berlie[1]

[1]Institute of Geosciences, Johannes Gutenberg-University Mainz, Mainz, Germany, [2]Institute of Geophysics, ETH Zürich, Zurich, Switzerland

The occurrence of large voluminous volcanic eruptions, so called caldera-forming eruptions, pose a threat to humankind and its growing cities located near volcanoes. With today's technology, the underlying processes of large scale magmatic systems can be modelled to further improve the understanding of all phases of an eruption. For those caldera-forming events, the deficit in overpressure and magma stored within the chamber results in a collapse of the ceiling and permanently alters the geomorphology of the region.

The processes of magma accumulation, the resulting overpressure and fracturing of the country rock can be modelled using various dynamic magma models. In this study we take a multiphysical approach and apply an open source thermal evolution magma intrusion model and couple it with a pseudo-transient Stokes solver (PT Solver) written in Julia. The model is set up to run in parallel and work on graphics processing unit (GPU) to maximise its efficiency and applicability to the newest generation of high performance computing (HPC) machines. The coupling enables us to model the growth of the magmatic system while also accounting for different complexities in rheology. The model provides an indication on the long-term magmatic evolution, both thermal and volumetric, during the build-up stage prior to caldera-forming eruptions.

AWP-ODC: A Highly Scalable HPC Tool for Dynamic Rupture and Wave Propagation Simulations

Kim Olsen[1], Daniel Roten[2], Te-Yang Yeh[1], Ke Xu[1], and Yifeng Cui[2]

[1]San Diego State University, [2]San Diego Supercomputer Center

AWP-ODC is an open-source dynamic rupture and wave propagation code which solves the 3D velocity-stress wave equation explicitly by a staggered-grid finite-difference method with fourth-order accuracy in space and second-order accuracy in time. The code is memory-bandwidth, with excellent scalability up to full machine scale on CPUs and GPUs, tuned on CLX, with support for generating vector folded finite difference stencils using intrinsic functions. AWP-ODC includes frequency-dependent anelastic attenuation Q(f), small-scale media heterogeneities, support for topography, Drucker-Prager visco-plasticity, and a multi-yield-surface, hysteretic (Iwan) nonlinear model using an overlay concept. Support for a discontinuous mesh is available for increased efficiency. An important application of AWP-ODC is the CyberShake Strain-Green-Tensor (SGT) code used for probabilistic hazard analysis in CA and other regions.

Here, we summarize implementation and verification of some of the widely-used capabilities of AWP-ODC, as well as validation against strong motion data and recent applications for future earthquake scenarios. We show for a M7.8 dynamic rupture ShakeOut scenario on the southern San Andreas fault that while simulations with a single yield surface reduces long period ground motion amplitudes by about 25% inside a wave guide in greater Los Angeles, multi-surface Iwan nonlinearity further reduces the values by a factor of two. In addition, we show assembly and calibration of a 3D Community Velocity Model (CVM) for central and southern Chile as well as Peru. The CVM is validated for the 2010 M8.8 Maule, Chile, earthquake up to 5 Hz, and the validated CVM is used for scenario simulations of megathrust scenario events with magnitude up to M9.5 in the Chile-Peru subduction zone for risk assessment.

Finally, we show simulations of 0-3 Hz 3D wave propagation for the 2019 Mw 7.1 Ridgecrest earthquake including a data-constrained high-resolution fault-zone model. Our results show that the heterogeneous near-fault low-velocity zone inherent to the fault zone structure significantly perturbs the predicted wave field in the near-source region, in particular by more accurately generating Love waves at its boundaries, in better agreement with observations, including at distances 200+ km in Los Angeles.

Tandem: A discontinuous Galerkin method for sequences of earthquakes and aseismic slip on multiple faults using unstructured curvilinear grids

Casper Pranger[1], Dave A. May[2], and Alice-Agnes Gabriel[1,2]

[1]LMU Munich, dept. of earth and environmental sciences, [2]Scripps institution of oceanography, UC San Diego

Seismic cycle modeling has advanced to the point where 3D models could be connected to geodetic and seismic observations to test hypotheses about controls on the depth and along-strike extent of ruptures, and interactions between seismic and aseismic slip events in geometrically complex fault systems. Such an undertaking does however require a greater degree of geometrical flexibility, material behaviors, code performance, and community participation than has so far been the standard.

In this light we present tandem, an open-source C++ code for 3D earthquake sequence modeling (Uphoff et al., 2022a). Tandem solves the elasticity problem with a discontinuous Galerkin finite element method on unstructured tetrahedral meshes. It can handle multiple, nonplanar faults and spatially variable elastic properties (Figure 1). The method can be extended to nonlinear off-fault material response (e.g., power-law viscoelasticity). The code is parallelized with MPI and uses the PETSc-TAO library (Balay et al., 2022) for time-integrators and preconditioned Krylov methods to solve the static elasticity problem. Faults are governed by rate- state friction and adaptive time-stepping permits modeling of dynamic rupture, the postseismic period, and interseismic loading, all across multiple earthquake cycles. The code is developed with best practices for open-source community software and includes documentation and tutorials to facilitate use by the community (github.com/TEAR-ERC/tandem).

Uphoff, C., D. A. May, and A.-A. Gabriel (2022a), A discontinuous Galerkin method for sequences of earthquakes and aseismic slip on multiple faults using unstructured curvilinear grids, Geophysical Journal International.
Balay, S., et al. (2022), PETSc/TAO users manual, Tech. rep., Argonne National Lab., Argonne, IL, USA (petsc.org/).

SESSION 2 EDGE-TO-END DATA WORKFLOW

KEYNOTE SPEAKER

Preparing Seismic Applications for Exascale Using Scientific Workflows

Scott Callaghan[1], Philip Maechling[1], Karan Vahi[2], Ewa Deelman[2], Fabio Silva[1], Kevin Milner[1], Kim Olsen[3], Robert Graves[4], Thomas Jordan[5], and Yehuda Ben-Zion[1]

[1]Argonne National Laboratory · [2]Lawrence Berkeley National Laboratory · [3]University of Colorado Boulder [4]University at Buffalo · [5]Tech-X Corporation · [6]University of Chicago · [7]Technische Universität Wien [8]Flatiron Institute· [9]King Abdullah University of Science & Technology (KAUST)

Scientific workflows are key to supporting the execution of large-scale simulations in many scientific domains, including solid earth geophysics. Although many different workflow tools exist, they share common features, enabling application developers to express their simulations as a series of linked software elements with data dependencies and then execute the workflow efficiently on distributed resources.

To illustrate the use and benefits of scientific workflows in seismic applications, this talk will describe CyberShake, a probabilistic seismic hazard analysis (PSHA) platform developed by the Southern California Earthquake Center (SCEC). CyberShake uses 3D physics-based wave propagation simulations with reciprocity to calculate ground motions for events from an earthquake rupture forecast (ERF). Typically, CyberShake considers over 500,000 events per site of interest, and then combines the individual ground motions with probabilities from the ERF to produce site-specific PSHA curves. CyberShake has integrated modules from another SCEC workflow application, the Broadband Platform (BBP), enabling CyberShake simulations to include both low-frequency deterministic and high-frequency stochastic content. This talk will discuss the workflow framework that CyberShake utilizes to support campaigns requiring hundreds of thousands of node-hours over months of wall clock time, and the lessons learned through 15 years of CyberShake simulations.

This talk will also reflect on the growth and development of workflow-based simulations and explore the challenges faced by applications in the exascale era, such as managing massive volumes of data, taking full advantage of exascale systems, and the emergence of AI-informed simulations. The talk will discuss ways in which workflow technologies may help mitigate these challenges as we move our science forward.

SHORT TALKS

BackTrackBB workflow for seismic source detection and location with PyCOMPSs parallel computational framework

Natalia Poiata[1,2], Javier Conejero[3], Rosa M. Badia[3], and Jean-Pierre Vilotte[4]

[1]National Institute for Earth Physics, Măgurele, Romania, [2]International Seismological Centre, UK
[3]Department of Computer Sciences, Barcelona Supercomputing Center (BSC-CNS), Barcelona, Spain, [4]Université Paris Cité, Institut de Physique du Globe de Paris, CNRS-INSU, Paris, France

In this work we present a scalable parallelization with PyCOMPSs (Tejedor et al., 2017; the Python binding of COMPSs) of the Python-based workflow BackTrackBB (Poiata et al., 2016) for the automatic detection and location of seismic sources using continuous waveform data recorded by regular to large seismic networks. PyCOMPSs is a task-based programming model for Python applications that relies in a powerful runtime able to extract dynamically the parallelism among tasks and execute them in distributed environments (e.g., HPC Clusters, Cloud infrastructures, etc.) transparently to the users. BackTrackBB with PyCOMPSs implementation allows to fully parallelize the seismic source detection and location process making it efficient and portable in terms of the use of available HPC resources.

We provide details of the BackTrackBB workflow implementation with PyCOMPSs and discuss its performance by presenting the results of the scalability tests and memory usage analysis. All the tests have been performed on the MareNostrum4 High-Performance computer of the Barcelona Supercomputing Centre. The first version of the BackTrackBB with PyCOMPSs workflow was developed in the context of the European Centre Of Excellence (CoE) ChEESE for Exascale computing in solid earth sciences. The initial workflow developments and performance tests made use of a simplified synthetic dataset emulating a large-scale seismic network deployment in a seismically active area and corresponding to 100 vertical sensors recording a month of continuous waveforms at a sampling rate of 100 sps. In the following testing step, the workflow was applied to the real-case two-month long dataset from Vrancea seismic region in Romania (corresponding to the 60-190 km deep earthquakes activity). Real seismic data scenario proved to present some challenges in terms of the data-quality control, that often occurs in the case of continuous waveforms recorded by the seismic observatories. This issue have been resolved and corresponding modifications were included in the final version of BackTrackBB with PyCOMPSs. The real dataset tests showed that the workflow allows improved detection and location of seismic events through the efficient processing of the large continuous seismic data with important performance and scalability improvements.

We show that BackTrackBB with PyCOMPSs workflow enables generation of fully reproducible, seismic catalogues (or seismic catalogues realizations) through the analysis of the continuous large (in terms of the number

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of seismic stations, data record length and covered area) seismic data-sets

Such implementations making use of advances full-waveform detection and location methods are currently highly-challenging or, some-times, impossible due to the amount of required main memory or unfeasible time to solution. PyCOMPSs has demonstrated to be able to deal with both issues successfully allowing to explore in greater depth the usage with BackTrackBB method. Workflows such as BackTrackBB with PyCOMPSs has the ability to significantly improve the detections and location process that is currently in place at seismological observatories or network operation centres, providing fully reproducing detailed catalogues in the seismically-active regions and allowing multiple input parameters testing (e.g., station configuration, velocity models).

ML Emulation of High Resolution Inundation Maps for Probabilistic Tsunami Hazard Analysis

Steven Gibbons, Erlend Storrøsten, and Finn Løvholt

NGI, Klimatilpasning og hydrodynamikk, Oslo, Norway

Local Probabilistic Tsunami Hazard Analysis (PTHA) aims to quantify the likelihood of a given metric of tsunami inundation at a given location over a given time interval. Seismic PTHA can require the simulation of thousands to tens of thousands of earthquake scenarios and can become computationally intractable when inundation over high-resolution grids is required. The numerical tsunami simulations write out time-series at offshore locations to simulate the wave height that would be recorded on tide gauges at selected locations.

The offshore time-series can be calculated at a fraction of the cost of the full inundation calculations. For a stretch of the coast of Eastern Sicily, we explore the extent to which a machine learning procedure trained on a small fraction of the total number of scenarios can predict the inundation map associated with a given offshore time-series.
We exploit a set of over 30000 numerical tsunami simulations to train and evaluate the ML-procedure. The ML-based inundation predictions for locations close to the water's edge, which are flooded in many of the scenarios, show excellent correspondence with the numerical simulation results.

Predicting inundation at locations further inland, which are flooded in only a small number of the simulations, is more challenging. Mitigating this shortcoming is a priority in the ongoing study.

Improving Probabilistic Gas Hazard Assessment through HPC: Unveiling VIGIL-2.0, an automatic Python workflow for probabilistic gas dispersion modelling

Silvia Massaro[1,2], Fabio Dioguardi[1,3], Alejandra Guerrero[4], **Antonio Costa**[2], Arnau Folch[4], Roberto Sulpizio[1,2], Giovanni Macedonio[5], and Leonardo Mingari[6]

[1]Instituto Superior Tecnico, Universidade de Lisboa, CERIS, Lisboa, Portugal, [2]CERIS - Civil Engineering Research and Innovation for Sustainability, Lisboa, Portugal, [3]Zhejiang University, Hangzhou, P.R. China, visiting at CERIS, Lisboa, Portugal, [4]Zhejiang University, Hangzhou, P.R. China

The atmospheric dispersion of gases (of natural or industrial origins) can be very hazardous to life and the environment if the concentration of some gas species overcome specie-specific thresholds. In this context, the natural variability associated to the natural phenomena has to be explored to provide robust probabilistic gas dispersion hazard assessments.

VIGIL-1.3 (automatic probabilistic VolcanIc Gas dIspersion modeLling) is a Python simulation tool born to automatize the complex and time-consuming simulation workflow required to process a large number of gas dispersion numerical simulations. It is interfaced with two models: a dilute (DISGAS) and a dense gas (TWODEE-2) dispersion model. The former is used when the density of the gas plume at the source is lower than the atmospheric density (e.g. fumaroles), the latter when the gas density is higher than the atmosphere and the gas accumulates on the ground and may flow due to the density contrast with the atmosphere to form a gravity current (e.g. cold CO2 flows).

In the enhancement of the code towards a higher-scale computing, here we present the ongoing improvements aimed to extend some code functionalities such as memory management, modularity revision, and full-ensemble uncertainty on gas dispersal scenarios (e.g. sampling techniques for gas fluxes and source locations).

Optimizations are also provided in terms of tracking errors, redesignation of the input file, validation of data provided by the users, and addition of the Latin hypercube sampling (LHS) for the post-processing of model outputs.

All these new features will be issued in the future release of the code (VIGIL-2.0) in order to facilitate the users which could run VIGIL on laptops or large supercomputer, and to widen the spectrum of model applications from routinely operational forecast of volcanic gas to long-term hazard and/or risk assessments purposes.

A first look at the calibration of near-fault motion models to synthetic big data from CyberShake's application to the Southwest Iceland transform zone

Farnaz Bayat[1], Milad Kowsari[1], Otilio Rojas[3], Marisol Monterrubio-Velasco[3], Josep de la Puente[3], and Benedikt Halldorsson[1,2]

[1]Faculty of Civil and Environmental Engineering, School of Engineering and Natural Sciences, University of Iceland, Reykjavik, Iceland, [2]Volcanic activity, earthquakes and deformation dept., Service and research Division, Icelandic Meteorological Office, Reykjavik, Iceland, [3]Barcelona Supercomputing Center (BSC-CNS), Barcelona, Spain

The strongest earthquakes in Iceland take place in its two large transform zones, the largest being up to magnitude 7.1. As a result, the earthquake hazard in Iceland is the highest in the transform zone. The capital region along with multiple small towns are either in close proximity or on top of the Southwest Iceland transform zone. As a result, the seismic risk is the highest in this region. A new physical 3D finite-fault system model has been developed that model strike-slip faulting in the transform zone as occurring on an array of north-south, near-vertical, dextral strike-slip faults and distributed along the entire transform zone with inter-fault distances ranging from 0.5-5 km. It is well-established that for near-vertical strike-slip faults, large-amplitude and long-period velocity pulses are found in the direction parallel and normal to the fault strike, respectively. The former is due to permanent tectonic displacement as a result of fault slip, and the latter is due to directivity effects. While the former is concentrated in close proximity to the fault and in particular the location of largest subevent of slip on the fault, the directivity pulse is found close to the fault ends and further away along the strike direction, either away from one end or both depending on if the fault rupture is uni- or bilateral, respectively. The forward directivity effect is generally considered to be the most damaging feature of the ground motions, particularly for long-period structures in the near-fault region.

The recorded near-fault data in Iceland, however, is relatively sparse, making it difficult to accurately capture the physical characteristics of near-fault ground motions. However, in the ChEESE project we have implemented the new 3D finite-fault system into the CyberShake simulation platform and applied in the kinematic rupture modelling and the corresponding ground motion time history simulation. As a result, we have produced a vast dataset of synthetic ground motion time histories for Southwest Iceland. The synthetic dataset now contains near all possible permutations of near-fault effects and will now be parametrized to reveal the scaling of key near-fault ground motion parameters (e.g., amplitude of pseudo-acceleration spectral, peak ground velocity, and the period of the near-fault pulses) associated with the source (fault slip distribution, and fault plane geometry). This parametrization will increase our understanding of near-fault ground motion and allow the development of simple, but physically realistic near-fault GMM that find practical application in physics-based PSHA.

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The Collaborative Seismic Earth Model: Generation 2

Sebastian Noe, Dirk-Philip van Herwaarden, Sölvi Thrastarson, and Andreas Fichtner

Institute of Geophysics, ETH Zurich, Zurich, Switzerland

We present the second generation of the Collaborative Seismic Earth Model (CSEM), a multi-scale global tomographic Earth model that continuously evolves via successive regional and global-scale refinements. Given finite computational resources, a systematic community effort enables the Earth model construction within the CSEM-architecture. It thereby takes advantage of the distributed human and computing power within the seismological community. The basic update methodology utilizes the current version of the CSEM as the initial model for regional tomographies. This setup allows to consistently incorporate previously accumulated knowledge into each new iteration of the CSEM.

The latest generation of the CSEM includes 21 regional refinements from full seismic waveform inversion, ranging from several tens of kilometers to the entire globe. Some noticeable changes since the first generation include detailed local waveform inversions for the Central Andes, Iran, South-east Asia and the Western United States, continental-scale refinements for Africa and Asia and a global long-period tomography in areas that are not included in any of the submodels. Across all regional refinements in the current CSEM, three-component waveform data from 1,637 events and over 700,000 unique source-receiver pairs are utilized to resolve subsurface structure. Minimum periods of models range between 8 and 55 seconds.

Using this model as a starting point, a global full-waveform inversion over multiple period bands down to periods of 50 seconds is deployed to ensure that the regional updates predict waveforms and that whole-Earth structure is honored. In this contribution, we will present the CSEM updating scheme and its parameterization, as well as the current state of the model. We show that the model predicts seismic waveforms on global and regional scales.

Active participation in the project is encouraged.

Volcanic ash dispersal and deposition workflow on HPC

Alejandra Guerrero, Arnau Folch, and Leonardo Mingari

Geosciences Barcelona (GEO3BCN-CSIC), Barcelona, Spain

DT-GEO is a project proposed to deal with natural or anthropogenically induced geohazards (earthquakes, volcanoes, landslides and tsunamis) by deploying a Digital Twin of the planet. The prototype will provide a way to visualize, manipulate and understand the response to hypothetical or on-going events by integrating data acquisition and models.

Due to the complexity of the development, the project has been divided into different work packages and components. The volcanic phenomena package includes 4 Digital Twin Components (DTCs): volcanic unrest, volcanic ash clouds and ground accumulations, lava flows, and volcanic gas dispersal. The volcanic ash and dispersal deposition component implements a workflow for atmospheric dispersal and ground deposition forecast systems. The workflow is composed of four general units.

The first one is the Numerical Weather Prediction (NWP) acquisition (provided by external institutions) refers to both: automatic obtention of the forecast (up to few days ahead) or the reanalysis (preprocess data from the past) in global or regional scales at different resolutions. Then, the Triggering and Eruption Source Parameters (ESP) is based on predefined communications channels and prioritized by an accuracy rank. The FALL3D model setup and run ensemble simulations, resulting from perturbing ESP values within a range. Finally, the postprocess refers to the compilation of the simulations into hazard maps.

Machine Learning based Estimator for ground Shaking maps

Marisol Monterrubio-Velasco[1], David Modesto[1], Scott Callaghan[2], and Josep de la Puente[1]

[1]Barcelona Supercomputing Center (BSC-CNS), Barcelona, Spain, [2]Southern California Earthquake Center, University of Southern California

Large earthquakes are among the most destructive natural phenomena. After a large-magnitude event occurs, a crucial task for hazard assessment is to rapidly and accurately estimate the ground shaking intensities in the affected region. To satisfy real-time constraints, ground shaking is traditionally evaluated with empirical relations called Ground Motion Prediction Equations (GMPE) which can be combined with local amplification factors and early data recordings, when available. Given their nature, GMPEs can be inaccurate to model rarely observed earthquakes, such as large earthquakes. Furthermore, even for very populated databases, GMPEs are characterized by large variances, as earthquakes of similar magnitude and location may have very different outcomes related to complex fault phenomena and wave physics.

The ML Estimator for Ground Shaking maps (MLESmap) workflow is proposed as a novel procedure that exploits the predictive power of ML algorithms to estimate ground acceleration values a few seconds after a large earthquake occurs. The inferred model can produce peak (spectral) ground motion maps for quasi-real-time applications. Due to its fast assessment, it can further be used to explore uncertainties quickly and reliably. MLESmap is based upon large databases of physics-based seismic scenarios to feed the algorithms.

Our approach (i.e. simulate, train, deploy) can help produce the next generation of ground shake maps, capturing physical information from wave propagation (directivity, topography, site effects) at the velocity of simple empirical GMPE. In this work, we will present the MLESmap workflow, its precision, and a use case.

A new Near-Fault Earthquake Ground Motion Model for Iceland from Bayesian Hierarchical Modeling

Farnaz Bayat[1], Milad Kowsari[1], Otilio Rojas[3], Marisol Monterrubio-Velasco[3], Josep de la Puente[3], and Benedikt Halldorsson[1,2]

[1]Faculty of Civil and Environmental Engineering, School of Engineering and Natural Sciences, University of Iceland, Reykjavik, Icelan, [2]Volcanic activity, earthquakes and deformation dept., Service and research Division, Icelandic Meteorological Office, Reykjavik, Iceland
[3]Barcelona Supercomputing Center (BSC-CNS), Barcelona, Spain

The strongest earthquakes in Southwest Iceland take place on a large number of North-South near-vertical dextral strike-slip faults located side-by-side along the entire zone. The capital region along with multiple small towns are in close proximity or on top of this fault system, along with all infrastructure and lifelines of our modern society. As a result, seismic hazard is the highest in this region and performing a probabilistic seismic hazard assessment (PSHA) as the most used procedure to reduce the ruinous effects of large earthquakes is vital.

A reliable PSHA requires a reliable ground motion models (GMMs) that can appropriately describe the ground shaking at any given location. However, past PSHA efforts in Iceland did not account for the complex near-fault effects in the form of long-period, high-amplitude velocity pulses that are the most damaging feature of ground motions in the near-fault region. Recently, a new 3D finite-fault system model of the entire bookshelf zone has been proposed for Southwest Iceland.

The model has been balanced against the rate of the tectonic plate motions and its seismic activity has been shown to be variable along the entire zone. Given the unknown fault locations, the model allows both for deterministic and random fault locations, and each fault is completely specified in terms of its maximum magnitude, its dimensions and its long-term slip and moment rate. In collaboration with ChEESE project, a realization of a 3000-year finite-fault earthquake catalogue based on the 3D finite-fault system model has been implemented in the CyberShake platform and the ground motion of each earthquake have been simulated for a dense grid of 594 stations. The simulation has been carried out on high-performance computing systems of the Barcelona Supercomputing Centre in Spain.

The variation of hypocentral locations and slip distribution on each finite-fault has produced 18 million event-station pairs of synthetic two-horizontal-component low-frequency ground motion time histories that have just become available, those that are simulated less than 40 km from the faults contain near-fault high-amplitude velocity pulses at larger magnitudes, where actual data is nonexistent in Iceland (i.e., above 6.5). Therefore, the purpose of this study is to use a new and vast near-fault dataset of synthetic ground motions to develop a near-fault GMM using an advanced Bayesian Hierarchical Modeling (BHM) for Southwest Iceland.

Characterization of Earthquake Near-fault Ground Motion Parameters Using an Artificial Neural Network on Synthetic Big Data

Milad Kowsari[1], Manuel Titos[2], Farnaz Bayat[1], Carmen Benitez[2], Marisol Monterrubio-Velasco[3], Otilio Rojas[3], Josep de la Puente[3], and Benedikt Halldorsson[1,4]

[1]Faculty of Civil and Environmental Engineering, School of Engineering and Natural Sciences, University of Iceland, Reykjavik, Iceland, [2]Department of Signal Theory, Telematics and Communications, University of Granada, Granada, Spain, [3]Barcelona Supercomputing Center (BSC-CNS), Barcelona, Spain [4]Volcanic activity, earthquakes and deformation dept., Service and research Division, Icelandic Meteorological Office, Reykjavik, Iceland

The South Iceland Seismic Zone (SISZ) and Reykjanes Peninsula Oblique Rift (RPOR) in Southwest Iceland together form one of the two major transform zones in the country that have the greatest capacity for the occurrence of destructive earthquakes. Therefore, in these regions, the seismic hazard is highest and performing a probabilistic seismic hazard assessment (PSHA) is vital as the foundation of earthquake resistant building design and seismic risk mitigation. It is well known both from observations as well as physics-based (PB) modeling of earthquake rupture and near-fault ground motion simulations, that the most damaging part of near-fault seismic motion is the velocity pulse, the large-amplitude and long-period pulse-like ground motions found along the fault and away from the ends of strike-slip faults. Such motions cause intense earthquake action primarily on large buildings, such as hydroelectric power plants, dams, powerlines, bridges and pipelines. However, the data is still too limited to enable the reliable calibration of a physically realistic, yet parsimonious, near-fault model that incorporate such effects into empirical ground motions models (GMMs), thereby allowing their incorporation into a formal PSHA. However, in the recent European H2020 ChEESE project, we established a new 3D finite-fault system model for the SISZ-RPOR system that now has facilitated the simulation of finite-fault earthquake catalogues.Moreover, the hypocentral locations and slip distributions on each synthetic fault have been varied, resulting in approximately 1 million earthquake-station-specific pairs of synthetic low-frequency and high-amplitude near-fault ground motion time histories. In this study, we analyse this dataset using an artificial neural network to reveal its characteristics in terms of amplitudes and the characteristics of near-fault velocity pulses, capturing all key features of such effects. The results will facilitate the incorporation of the near-fault effects into new near-fault and far-field GMMs, that are a key element of conventional PSHA. This will both enable the near-fault PB-PSHA along with the comparison of PSHA from the synthetic dataset vs. the GMMs. This will usher in a new era of PB-PSHA in Iceland.

Towards physics-based finite-fault Monte Carlo PSHA for Southwest Iceland based on a new fault system model

Milad Kowsari[1] and **Benedikt Halldorsson**[1,2]

[1]Faculty of Civil and Environmental Engineering, School of Engineering and Natural Sciences, University of Iceland, Reykjavik, Iceland, [2]Volcanic activity, earthquakes and deformation dept., Service and research Division, Icelandic Meteorological Office, Reykjavik, Iceland

Throughout history, damaging earthquakes have repeatedly struck in Southwest Iceland, the country’s most populated and seismically active region. There, the interplate earthquakes do not occur on sinistral strike-slip faults parallel to the plate margin, but instead on a dense array of near-vertical dextral faults striking perpendicular to the plate margin. This “bookshelf” faulting has not explicitly been accounted for in probabilistic seismic hazard assessment (PSHA). Instead, incomplete earthquake catalogues and simplistic seismic sources have been used in past PSHA that have used conventional methods. Recently however, a new and physics-based 3D fault system model of the Southwest Iceland transform zone has been proposed that effectively explains the observed Icelandic earthquake catalogues. The model moreover allows the systematic spatial variation of fault slip-rates to be modeled by discrete subzonation of the fault system and the equivalent parameters of seismic activity (Mmax, a- and b-values). Through random realizations of fault locations as postulated by the new model, we have simulated multiple finite-fault earthquake catalogues for the entire bookshelf system for earthquakes ranging from magnitude 4 to 7.

This in fact allows us to apply conventional PSHA but instead of using e.g.

seismic point sources distributed over a designated seismic source areas, the seismic activity of which is predicted by limited historical catalogues, the synthetic finite-fault catalogues are time-independent and embody fully the first two key elements of PSHA, the seismic source locations along with their activity rates. Using multiple empirical hybrid Bayesian ground motion models (GMMs) that recently have been proposed for Southwest Iceland we have predicted the amplitudes (peak ground accelerations and pseudo-acceleration spectral response) from each synthetic finite-fault earthquake on a grid of hypothetical stations. This enables us to carry out a Monte Carlo PSHA that is based on a physical earthquake fault system model. We present the provisional PSHA results for Southwest Iceland and compare them to other relevant efforts, the Icelandic National Annex to Eurocode 8 and the ESHM20, but most importantly to those of a parallel study that carries out a physics-based PSHA based on synthetic ground motion time histories (on the same hypothetical network) from kinematic earthquake rupture modeling (on the same finite-fault earthquake catalogues) implemented in the CyberShake framework adapted to the Southwest Iceland tectonic situation and earthquake source scaling.

Monitoring the sediment dynamics of Maltese beaches. The SIPOBED project and its future challenges.

Luciano Galone[1], Emanuele Colica[1,2], Peter Iregbeyen[1], Luca Piroddi[1], Deidun Alan[1], Gianluca Valentino[1], Adam Gauci[1], and Sebastiano D’Amico[1]

[1]Department of Geosciences, University of Malta. Msida, Malta, [2]Research & Planning Unit, Ministry for public works and Planning, Malta. Floriana, Malta

Pocket beaches are small beaches bounded by natural promontories, free from direct sedimentary inputs other than those coming from the erosion of their cliffs.

Malta's pocket beaches are one of the most significant geomorphological features of the archipelago. They play an important role for a variety of ecological and economic reasons. Sediment dynamics (mainly sand) is one of the most relevant factors to be considered in those beach system. As the pocket beach system behaves as an integrated unit, periodic bathymetric monitoring is essential - and challenging - from an environmental management perspective.

The SIPOBED project (Satellite Investigation to study POcket BEach Dynamics) develops an integrated tool capable of monitoring sediment dynamics using SAR and digital photogrammetry to monitor beach topographic variations and multispectral UAV and satellite images to derive bathymetry.

Obtaining updated in situ bathymetric measurements is essential to calibrate and re-calibrate the model over time and conduct more actualized and accurate multispectral-derived bathymetry.

In this context, the collection of data by citizens, for instance, bathymetric data collected by private boats abundant in the archipelago, in conjunction with the processing power of modern computing, represents the new challenge of Maltese pocket beach monitoring. The SIPOBED project is financed by the Malta Council for Science and Technology (MCST, https://mcst.gov.mt/) through the Space Research Fund (Building capacity in the downstream Earth Observation Sector), a programme supported by the European Space Agency.

Real time Earthquake detection using Deep Learning

Wei Li[1], Megha Chakraborty[1,2], Georg Rümpker[1,2], and **Nishtha Srivastava**[1,2]

[1]Frankfurt Institute of Advanced Studies, Ruth-Moufang-Str. 1, 60438 Frankfurt am Main, Germany,
[2]Institute of Geosciences, Goethe-University Frankfurt, 60438 Frankfurt am Main, Germany

Seismic event detection and its magnitude estimation are the two crucial steps in real-time earthquake monitoring and early warning systems. Traditional EEW systems can be limited in their ability to accurately detect the arrival phases (P and S waves) and locate earthquakes, particularly for events with high levels of background noise. Deep learning has emerged as a promising alternative to traditional EEW algorithms, since these algorithms can automatically learn complex patterns and features in seismic data, allowing them to more accurately detect the seismic phase arrival times in the signals.

In this study, we first propose a deep learning based architecture DynaPicker which uses a dynamic convolutional neural network to detect seismic body wave phases. Then, the pre-trained model is used to pick the seismic phases on the continuous seismic recording. This model is further combined with another deep-learning model CREIME to perform magnitude estimation. The experimental results on several open-source seismic datasets demonstrate that DynaPicker achieved a higher testing accuracy in seismic phase identification compared to other benchmark models. Additionally, DynaPicker's robustness in classifying seismic phases was tested on the low-magnitude seismic data polluted by noise. DynaPicker can be adapted to handle input data of varying lengths, making it well-suited for P/S phase picking. When applied to continuous seismic data, DynaPicker can identify more seismic events accurately and produce lower arrival time picking errors than baseline methods. We also found that using the estimated P-phase arrival time of DynaPicker, the CREIME model shows reliable results in estimating the magnitude of the aftershocks of the Turkey earthquake.

SESSION 3 STATE-OF-THE-ART IN COMPUTATIONAL GEOSCIENCES

KEYNOTE SPEAKER

Simulation of Geological CO2 Storage with the GEOS Open-Source Multiphysics Simulator

Nicola Castelletto

Lawrence Livermore National Laboratory

Carbon capture and storage (CCS) is one of the most important technologies to achieve large-scale reduction in global carbon dioxide (CO2) emissions. The essence of CCS is to capture CO2 produced at power plants and industrial facilities and transport it to safe, permanent storage deep underground. Reducing CO2 emissions into the atmosphere is crucial to cut the carbon footprint of our society. The evaluation of CO2 storage candidate sites requires predictive simulation capabilities to assess site capacity and safety.

We present an overview of the GEOS multiphysics simulation platform, an open-source simulator capable of serving as the computational engine for CCS evaluation workflows. We will discuss the development path of GEOS, and motivations to transition from a collection of smaller single-institution code development efforts to a multi-institution collaboration. We will describe the development of a discretization-data infrastructure, a standardized approach to solving single and coupled physics problems, and a strategy to achieve reasonable levels of performance portability across hardware platforms. We will outline the approach to documentation, and planned method of user interaction as the growth of that user base accelerates.

SHORT TALKS

HPC projects in the Solid Earth ecosystem

Arnau Folch

Geosciences Barcelona (GEO3BCN-CSIC), Barcelona, Spain

The second phase (2023-2026) of the EuroHPC Center of Excellence for Exascale in Solid Earth (ChEESE-2P), funded by HORIZON-EUROHPC-JU-2021-COE-01 under the Grant Agreement No 101093038, will prepare 11 European flagship codes from different geoscience domains. Codes will be optimised in terms of performance on different types of accelerators, scalability, containerisation, and continuous deployment and portability across tier-0/tier-1 European systems as well as on novel hardware architectures emerging from the EuroHPC Pilots (EuPEX/OpenSequana and EuPilot/RISC-V) by co-designing with mini-apps.

Flagship codes and workflows will be combined to farm a new generation of 9 Pilot Demonstrators (PDs) and 15 related Simulation Cases (SCs) representing capability and capacity computational challenges selected based on their scientific importance, social relevance, or urgency. On the other hand, the first phase of ChEESE was pivotal in leveraging an ecosystem of European projects and initiatives tackling computational geohazards that will benefit from current and upcoming exascale EuroHPC infrastructures. In particular, Geo-INQUIRE (2022-2024, GA No 101058518) and DT-GEO (2022-2025, GA No 101058129) are two on-going Horizon Europe projects relevant to the Solid Earth ecosystem.

The former will provide virtual and trans-national service access to data and state-of-the-art numerical models and workflows for monitoring and simulation of the dynamic processes in the geosphere at unprecedented levels of detail and precision. The later will deploy a prototype Digital Twin (DT) on geophysical extremes including 12 self-contained Digital Twin Components (DTCs) addressing specific hazardous phenomena from volcanoes, tsunamis, earthquakes, and anthropogenically-induced extremes to conduct precise data-informed early warning systems, forecasts, and hazard assessments across multiple time scales. All these initiatives liaise, align, and synergise with EPOS and longer-term mission-like initiatives like Destination Earth.

Complete workflow for tsunami simulation and hazard calculation in urgent computing using HPC services

Louise Cordrie[1], Jacopo Selva[1,2], Jorge Ejarque[3], Fabrizio Bernardi[4], Roberto Tonini[4], Jorge Macías Sánchez[5], Carlos Sánchez Linares[5], Steven Gibbons[6], and Finn Løvholt[6]

[1]Istituto Nazionale di Geofisica e Vulcanologia (INGV) [2]Sezione di Bologna, Italia University of Napoli (Universita degli Studi di Napoli Frederico II), Department of Earth, Environmental and Resource Sciences, Napoli, Italia [3] Barcelona Supercomputing Center (BSC-CNS), Barcelona, Spain [4]Istituto Nazionale di Geofisica e Vulcanologia (INGV) Sezione di Roma, Italia [5]University of Málaga (EDANYA, Faculty of Sciences), Málaga, Spain [6] Norwegian Geotechnical Institute (NGI), Oslo, Norway

Tsunami urgent computing procedures quantify the potential hazard due to a seismically-induced tsunami right after an earthquake, that is from minutes to a few hours. The hazard is quantified by simulating the tsunami from source to shore, taking into account the uncertainty in the source parameters and the uncertainty associated with the wave generation, propagation, and inundation.

In the European eFlows4HPC project, an HPC workflow for urgent computing of tsunami hazard assessment is currently being developed, consisting of the following steps: 1) retrieval of parameters for the tsunamigenic earthquake (magnitude, hypocentre and associated uncertainties), 2) definition of a seismic source ensemble, 3) simulation of the tsunami generated by each scenario in the ensemble, 4) aggregation of the results to produce an estimate of tsunami hazard, which also incorporates a basic treatment of uncertainty modelling and 5) update of the ensemble based on incoming data.

Initially implemented on the Power-9 machine at BSC, the workflow has been fully embedded into a PyCOMPSs framework that enables parallel task execution and integrates full tsunami simulations for the first time. The tsunami numerical model (Tsunami-HySEA) computes the tsunami from the source to coastal impact using nested grids with resolution from kilometres to meters. To limit the number of simulations and converge faster towards stable hazard estimates, new methods for defining the seismic source ensembles have been developed. When applied to several past earthquakes and tsunamis (e.g., the 2003 Boumerdes and the 2017 Kos-Bodrum earthquakes), our new sampling strategy yielded a reduction of 1 or 2 orders of magnitude for ensemble size, allowing a drastic reduction in the computational effort. This reduction may be exploited to improve tsunami simulation accuracy, increasing the computational effort available for each simulation for the same overall cost. The workflow also allows the integration of new incoming data (focal mechanism, seismic or tsunami records) for an “on the fly” update of the PTF based on this new information.

The improvement of the workflow through a well-defined ensemble of scenarios, realistic simulations and integration of incoming data, strongly reduces the uncertainty and yields to an update of the probabilistic forecasts without compromising theiraccuracy. This can be crucial in mitigating the risk far from the seismic source, and in improving risk management by better informing decision-making in an emergency framework.

Can we model lava flows faster than real-time to assist on a first volcanic emergency response?

Carlos Paredes[1], Marcos David Márquez[1], and Miguel Llorente[2]

[1]Universidad Politécnica de Madrid, School of Mines and Energy, Dpt. Geological & Mining Engineering, Spain, [2] Department of Geological Risks and Climate Change, Spanish Geological Survey (Centro Nacional Instituto Geológico y Minero de España, IGME) Consejo Superior de Investigaciones Científicas, CSIC

Remote sensing data and numerical simulation models of lava flows have been combined to assess the possibility of rapid, real-time response during the effusive crisis of the recent Cumbre Vieja (Sep 19 - December 13, 2021) eruptive episode. Here, we use the monitoring products openly distributed by COPERNICUS through the Emergency Management Service (EMSR546) and by the Cabildo Insular de la Palma (daily-updated polygons of the extent of the lava flow) and the lava flow emplacement as simulated with VolcFlow, during the first seven days of the eruption, and supported by the location of the effusive foci provided by the IGN.

The morphometric analysis of the satellite data has allowed us to estimate, assuming a non-Newtonian behaviour of the lava, the flows emitted, and their viscosities, using expressions based on the morphological dimensions, their advancing speed, and their density. The morphometric values thus obtained have been used as initial conditions for the numerical calibration, which has been done by minimising the Jaccard coefficient used as the objective function, but other geometric measures can be used as functionals to be minimised. Although we have designed and presented a task flow as a procedure to perform a dynamic numerical semiautomatic calibration over time of the rheological parameters necessary to simulate the day-to-day evolution of the lava flooding zone, based on the remote information recorded, for its validation we have carried out the search for the solution to the optimisation problem manually.

The results have allowed us to obtain a Jaccard coefficient between 85% and 60% with a calculation time, including calibration, of less than 7 days of simulated lava flow. Also, an emission rate of about 140 m3/s of lava flow has been estimated, during the first 24 h of the eruptive process, which decreased asymptotically to 60 m3/s. This value can be cross-checked with information from other remote sources using TADR.

Viscosity varied from 8 × 106 Pa s, or a yield strength of 42 × 103 Pa, in the first hours, to 4 × 107 Pa s and 35 × 103 Pa, respectively, during the remainder of the seven days. In addition, the modelling allowed mapping the likely evolution of the lava flow fields until 27 September, with an acceptable lava height distribution for the highest values and a Jaccard coefficient of 85%, in order to determine the behaviour of the available response time, according to the computational cost, for the numerical estimation of the rheology and to generate real-time forecasts of the evolution.

This integration of satellite data with numerical model calibration for parametric estimation of the La Palma 2021 eruption holds great promise for providing a real-time response system to other future volcanic eruptions and providing the necessary information, mainly in the form of dynamic evolution maps, for efficient emergency preparedness and management.

Modelling of extreme sea-level hazards: state-of-the-art and future challenges

Iva Tojčić, Cléa Denamiel, and Ivica Vilibić

Ruđer Bošković Institute, Laboratory for Physical Oceanography and Chemistry of Aquatic Systems, Croatia

Meteotsunami events – tsunami-like ocean waves driven by atmospheric disturbances – are, by nature, rare, specific to certain geographical regions and highly variable in time. Consequently, the coastal hazards due to these types of events are known to be difficult to forecast with state-of-the art numerical models presently applied around the world. In order to help the local communities to better prepare for these destructive events (e.g., set temporary protection against flooding and waves, avoid swimming, etc.) and minimize the losses, the Croatian Meteotsunami Early Warning System (CMeEWS) has been recently implemented in the Adriatic Sea in the testing mode. The CMeEWS is mostly based on the Adriatic Sea and Coast (AdriSC) modelling suite and uses an innovative deterministic-stochastic approach for extreme sea-level event predictions. It provides meteotsunami hazard forecasts depending on (1) daily deterministic forecasts by coupled kilometer-scale atmosphere-ocean models, (2) atmospheric observations and (3) stochastic forecasts of extreme sea-level distributions at endangered locations derived with a surrogate model approach. Some of these steps require substantial computational resources and needs an optimized data flow which, at end, defines the operability of the service.

Here, the advantages but also the drawbacks of such an approach will be presented through several applications of the AdriSC modelling suite during meteotsunami events in the Adriatic Sea. The future challenges concerning meteotsunami extreme sea-level modelling will be discussed and some potential avenues to further develop the model skills will be considered.

POSTERS

Three-dimensional, multiphase flow numerical models of phreatic volcanic eruptions

Tomaso Esposti Ongaro and Mattia de' Michieli Vitturi

Istituto Nazionale di Geofisica e Vulcanologia, Pisa, Italy

Explosive volcanic eruptions are characterized by the ejection in the atmosphere of volcanic gases and fragments of magma and/or lithics at high temperature, pressure and velocity. They encompass a broad range of magnitudes, with volumes of ejecta spanning from less than 106 m3, to 109-1011 m3 of Plinian eruptions, up to the largest known volcanic events, able to erupt up to thousands of km3 of magma. Phreatic eruptions are among the smallest in this range; they do not involve the eruption of fresh magma, but are instead triggered by a sudden rise of pressure and temperature in a shallow magmatic-hydrothermal system. Despite their relatively small size, phreatic eruptions are frequent on Earth and difficult to anticipate, and represent therefore a significant hazard, testified by the recent eruptions in Tongariro's Te-Maari crater (NZ, 2012), and during the tragic development of events in Ontake (JP, 2014) and Whakaari/White Island (NZ, 2019).

The main challenges of the numerical simulation of explosive volcanic phenomena have traditionally been identified in the complex fluid dynamics of polydisperse multiphase mixtures (with particle grains ranging from a few microns to metres) and in the extremely broad range of relevant dynamical scales characterizing compressible turbulent flows of gas and particles in the atmosphere. Three-dimensional, high-performance computer models based on different approximations of the multiphase flow theory have been designed to simulate the fluid dynamics of explosive eruptions, and to define hazard and impact scenarios. However, until now, it was difficult to quantify the uncertainty associated with numerical predictions.

We here discuss the present bottlenecks and challenges of the 3D modelling of phreatic volcanic eruptions in the quest for urgent definition of impact scenarios and probabilistic hazard assessment at Vulcano island (Aeolian archipelago, Italy). Exascale computing in these applications offers the opportunity to increase the complexity of the physical model (including new key processes as the flashing of liquid water), to describe the wide range of lithic fragments ejected during the eruption, to achieve unprecedently high spatial resolution at the source and close to the terrain, and to perform large ensembles of numerical simulations to quantify the epistemic uncertainty associated with the model initial and boundary conditions.

Challenges associated with the development, maintenance and porting on new HPC architectures of numerical models are finally discussed.

Hydro-mechanical modeling of injection-induced seismicity at the Deep Heat Mining Project of Basel, Switzerland

Auregan Boyet[1,2,3], Silvia De Simone[3], and Víctor Vilarrasa[1]

[1]Global Change Research Group (GCRG), IMEDEA, CSIC-UIB, Esporles, Spain, [2]Associated Unit: Hydrogeology Group (UPC-CSIC), [3]Institute of Environmental Assessment and Water Research (IDAEA), CSIC, Barcelona, Spain

Fluid injection in subsurface reservoirs often induces seismicity, which is a limiting factor in the deployment of geo-energies, as it is the case for Enhanced Geothermal Systems (EGS). EGS are commonly deep granitic reservoirs subject to hydraulic stimulation in order to enhance the fracture permeability and consequently the heat production. Injection-induced seismicity occurs also after the stop of injection, and in many cases the largest earthquakes occur after the shut-in. The counterintuitive post-injection large magnitude seismicity is still not well understood and its modelling is necessary to improve the understanding of the processes triggering the seismicity. Pressure-driven processes, as pore pressure increase and poroelastic stress/strain variations, have been identified as triggers of seismicity, together with stress interactions, thermal disparities and geomechanical interactions.

We design a coupled hydro-mechanical 2D model of the well-known case of post-injection induced seismicity of Basel EGS (Deep Heat Mining Project at Basel, Switzerland, 2006). We use CODE_BRIGHT, a finite element method software able to perform monolithic coupled thermo-hydro-mechanical analysis in geological media. The faults respond to a Mohr-Coulomb failure criterion with strain weakening and dilatancy, which allow to simulate fault reactivation and its aperture variation. The model is able to reproduce the pressure and stress variations, and the consequent fault reactivations through the simulations. The Basel EGS has been well documented and its characteristics are available. We are able to reproduce the spatio-temporal induced seismicity.

Yet, our current numerical method takes long computational time. To speed up simulations, we simplify the model geometry by grouping faults that yield similar static stress transfer, computed with the code Coulomb3, which solves an analytical solution to compute stress changes caused by fault slip. The combination of numerical with analytical solutions is an effective way of obtaining faster computing models. By simultaneously assimilating monitoring data in real-time with an efficient computing model would enable a better understanding of the fluid-injection effects on the stability of the reservoir, and potentially the mitigation of the induced seismicity.

A computationally efficient numerical model to understand potential CO2 leakage risk within gigatonne scale geologic storage

Iman R. Kivi[1,2,3], Roman Y. Makhnenko[4], Curtis M. Oldenburg[5], Jonny Rutqvist[5], and Victor Vilarrasa[3]

[1]Institute of Environmental Assessment and Water Research, Spanish National Research Council (IDAEA-CSIC), Barcelona, Spain [2]Associated Unit: Hydrogeology Group (UPC-CSIC), Barcelona, Spain [3]Global Change Research Group (GCRG), IMEDEA, CSIC-UIB, Esporles, Spain [4]Department of Civil & Environmental Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA [5]Energy Geosciences Division, Lawrence Berkeley National Laboratory, CA, USA

The majority of available climate change mitigation pathways, targeting net-zero CO2 emissions by 2050, rely heavily on the permanent storage of CO2 in deep geologic formations at the gigatonne scale. The spatial and temporal scales of interest to geologic carbon storage (GCS) raise concerns about CO2 leakage to shallow sediments or back into the atmosphere. The assessment of CO2 storage performance is subject to huge computational costs of numerically simulating CO2 migration across geologic layers at the basin scale and is therefore restricted in practice to multi-century periods. Here, we present a computationally affordable and yet physically sound model to understand the likelihood of CO2 leakage over geologic time scales (millions of years) (Kivi et al., 2022). The model accounts for vertical two-phase flow and transport of CO2 and brine in a multi-layered system, comprising a sequence of aquifers and sealing rocks from the crystalline basement up to the surface (a total thickness of 1600 m), representative of a sedimentary basin. We argue that the model is capable of capturing the dynamics of CO2 leakage during basin-wide storage because the lateral advancement of CO2 plume injected from a dense grid of wellbores transforms into buoyant vertical rise within a short period after shut-in.

A critical step in the proposed model is its initialization, which should reproduce the average CO2 saturation column and pressure profiles. We initialize the model by injecting CO2 at a constant overpressure into an upper lateral portion of the target aquifer while the bottom boundary is permeable to brine, resembling brine displacement by CO2 plume or leakage at basin margins. The optimum model setting can be achieved by adjusting the brine leakage parameter through calibration.

We solve the governing equations using the finite element code CODE_BRIGHT. Discretizing the model with 7,100 quadrilateral elements and using an adaptive time-stepping scheme, the CPU time for the simulation of CO2 containment in the subsurface for 1 million years is around 140 hours on a Xeon CPU of speed 2.5 GHz. The obtained results suggest that the upward CO2 flow in free phase is strongly hindered by the sequence of caprocks even if they are pervasively fractured. CO2 leakage towards the surface is governed by the intrinsically slow molecular diffusion process, featuring aqueous CO2 transport rates as low as 1 meter per several thousand years. The model shows that GCS in multi-layered geologic settings is extremely unlikely to be associated with leakage, implying that GCS is a secure carbon removal technology.

Tsunami risk management in the Exascale Era: Global advances and the European standpoint

Cláudia Reis[1], André R. Barbosa[2], Denis Istrati[3,4], Stephane Clain[5], Rui Ferreira[1], Luis Matias[6], and Erin Wirth[7]

[1]Lisbon University , Instituto Superior Técnico, Department of Civil Engineering, Environment and Georresources, Portugal [2] School of Civil and Construction Engineering, Oregon State University, Corvallis, Oregon, United States of America [3] School of Civil Engineering, National Technical University of Athens, Greece [4] Department of Civil and Environmental Engineering, University of Nevada Reno, United States [5]Department of Mathematics, Coimbra, Portugal [6]Instituto Dom Luiz, Faculdade de Ciências da Universidade de Lisboa, Lisboa, Portugal [7] USGS, Earthquake Science Center, United States

Regional and local tsunami sources are a cliché of scientific disaggregation. From the physical perspective, despite emerging studies on cascading hazard and risk, hazard characterization often sees the tsunami as an individual event without addressing the effects of the primary hazard (typically a high-magnitude earthquake) that triggered the tsunami. Moreover, tsunami effects are partitioned into single processes: hydraulic effects or induced effects, such as debris transport, which is a representative approach often assumed when treating complex phenomena. From a technical perspective, describing cascading hazards and translating them into a composite loading pattern for natural and built environments is challenging, and the difficulty increases exponentially when fluid-soil-interactions are considered. From a modeling perspective, physical and numerical simulations are employed to complement scarce databases of extreme tsunami events. However, the level of modeling sophistication deemed necessary to reproduce such complex phenomena is elevated and there are uncertainties associated with natural phenomena and their modelling, ranging from the genesis of the tsunami to structural and community response. The number and influencing potential of uncertainties pose an extraordinary concern when developing mitigation measures. From a risk management perspective, cascading natural and anthropogenic hazards constitutes a challenge for combining safety requirements with financial, social, and ecological concerns. Risk management can benefit from strengthening the ties between natural hazards and engineering practitioners, linking science and industry, and promoting dialogue between risk analysts and policy-makers.

Ultimately, risk management requires heterogeneous data and information from real and synthetic origins. Yet, the quality of data used for risk management may often depend on the computational resources (in terms of performance, energy, and storage capacity) needed to simulate complex multi-scale and multi-physics phenomena, as well as to analyze large data sets. For example, the quality of the numerical solutions is often dependent on the amount of data used to calibrate the models and the runtime of the models needs to be aligned with time constraints (ex.: faster than real time tsunami simulations for early warning systems). The North American platform Hazus is capable of producing risk maps. In the European risk assessment, there is a lack of integration and interaction of results from GEM and SERA, and TSUMAPS-NEAM projects, intended to develop seismic and tsunami hazard studies, respectively. The computational modeling aids in the advancement of scientific knowledge by aggregating the numerous factors involved and their translation to tsunami risk management policies.

A global trend in geosciences and engineering is to develop sophisticated numerical schemes and to build computational facilities that can solve them, thereby aiming to reduce uncertainty levels and preparing the scientific (r)-evolution for the so-called Exascale Era. The present work aims to gather multidisciplinary perspectives on a discussion about: 1) challenges to overcome on tsunami risk management, such as sophistication of earthquake and tsunami numerical schemes; 2) uncertainty-awareness and future needs to develop unanimous and systematic measures to reduce uncertainties associated with geophysical and engineering processes; 3) pros and cons of using HPC resources towards safety and operational performance levels; and 4) applicability to critical infrastructures.

Combining High-Performance Computing and Neural Networks for Tsunami Maximum Height and Arrival Time Forecasts

Juan Francisco Rodríguez Gálvez, Jorge Macías Sáncez, Manuel Jesús Castro Díaz, Marc de la Asunción, and Carlos Sánchez-Linares

University of Málaga, Departamento de Análisis Matemático, Estadística e Investigación Operativa y Matemática Aplicada, Spain

Operational Tsunami Early Warning Systems (TEWS) are crucial for mitigation and highly reducing the impact of tsunamis on coastal communities worldwide. In the North-East Atlantic, the Mediterranean, and connected Seas (NEAM) region, these systems have historically utilized Decision Matrices for this purpose. The very short time between tsunami generation and landfall in this region makes it extremely challenging to use real-time simulations to produce more precise alert levels and the only way to include a computational component in the alert was to use precomputed databases. Nevertheless, in recent years, computing times for a single scenario have been progressively reduced to a few minutes or even seconds depending on the computational resources available. In particular, the EDANYA group at the University of Málaga, Spain, has focused on this topic and developed the GPU code Tsunami-HySEA for Faster Than Real Time (FTRT) tsunami simulations. This code has been implemented and tested in TEWS of several countries (such as Spain, Italy, and Chile) and has undergone extensive testing, verification and validation.

In this study, we propose the use of neural networks (NN) to predict the maximum height and arrival time of tsunamis in the context of TEWS. The advantage of this approach is that the inference time required is negligible (less than one second) and that this can be done in a simple laptop. This allows to consider uncertain input information in the data and still providing the results in some seconds. As tsunamis are rare events, numerical simulations using the Tsunami-HySEA are used to train the NN model. This part of the workflow requires producing a large amount of simulations and large HPC computational resources must be used. We utilized the Tsunami-HySEA code and the Spanish Network for Supercomputing (RES), to apply neural networks (NN) and obtain the numerical results.

Machine learning (ML) techniques have gained widespread adoption and are being applied in all areas of research, including tsunami modeling. In this work, we employ Multi-Layer Perceptron (MLP) neural networks to forecast the maximum height and arrival time of tsunamis at specific locations along the Chipiona-Cádiz coast in Southwestern Spain. In the present work, initially several individual models are trained and we show that they provide accurate results. Then ensemble techniques, which combine multiple single models in order to reduce variance, are explored. The ensemble models often produce improved predictions.

The proposed methodology is tested for tsunamis generated by earthquakes on the Horseshoe fault. The goal is to develop a neural network (NN) model for predicting the maximum height and arrival time of such tsunamis at multiple coastal locations simultaneously. The results of our analysis show that deep learning is a promising approach for this task. The proposed NN models produce errors of less than 6 cm for the maximum wave height and less then 212 s for the arrival time for tsunamis generated on the Horseshoe fault in the Northeastern Atlantic.

Ash fallout long term probabilistic volcanic hazard assessment for Neapolitan volcanoes: an example of what Earth Scientists can do with HPC resources

Manuel Stocchi[1], Silvia Massaro[1,2], Beatriz Martínz Montesinos[2], Laura Sandri[2], Jacopo Selva[3], Roberto Sulpizio[1,2,4], Biagio Giaccio[4], Massimiliano Moscatelli[4], Edoardo Peronace[4], Marco Nocentini[4,5], Roberto Isaia[6], Manuel Titos Luzón[7], Pierfrancesco Dellino[1], Giuseppe Naso[8], and Antonio Costa[2]

[1] Università degli Studi Aldo Moro di Bari, Department of Earth and geo-environmental sciences, Italy, [2] Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Bologna, Italy, [3] Dipartimento di Scienze della Terra, dell'Ambiente e delle Risorse, Università Federico II, Napoli, Italy, [4]Istituto di Geologia Ambientale e Geoingegneria, Consiglio Nazionale delle Ricerche, Roma, Italy, [5]Dipartimento Servizio Geologico d'Italia, Istituto Superiore per la Protezione e Ricerca Ambientale, Rome, Italy, [6]Istituto Nazionale di Geofisica e Vulcanologia, Osservatorio Vesuviano, Napoli, Italy [7]Signal Processing and Machine Learning, University of Granada, Spain, [8]Dipartimento di Protezione Civile, Rome, Italy

The creation of hazard maps relative to volcanic phenomena requires taking into account the intrinsic complexity and variability of eruptions. Here we present an example of how HPC can allow producing a high resolution multi-source probabilistic hazard assessment due to tephra fallout over a domain covering Southern Italy.

The three active volcanoes in the Neapolitan area, Somma-Vesuvius, Campi Flegrei and Ischia, were considered as volcanic sources. For each one, we explored three explosive size classes (Small, Medium and Large) for Somma Vesuvius and Campi Flegrei, and one explosive size class (Large) for Ischia. For each size class, we performed 1500 numerical simulations of ash dispersion (total of 10500) using the Fall3D (V8.0) model over a computational domain covering Southern Italy with a 0.03° 0.03° (~3 km 3 km) resolution. Within each size class, the eruptive parameters have been randomly sampled from well-suited probability distributions and with different meteorological conditions, obtained by randomly sampling a day between 1990 and 2020 and retrieving the relative data from the ECMWF ERA5 database. This allowed exploring the intra-class variability and to quantify aleatoric uncertainty. The results of these simulations have been post-processed with a statistical approach by assigning a weight to each eruption (based on its eruption magnitude) and the annual eruption rate of each size class. For the case of Campi Flegrei, the variability in the eruptive vent position has also been explored by constructing a grid of possible vent locations with different spatial probability. By merging the results obtained for each source and size class we produced a portfolio of hazard maps showing the expected mean annual frequency of overcoming selected thresholds in ground tephra load. A disaggregation analysis has also been performed in order to understand which particular source and/or size class had the greater impact on a particular area.

The completion of this work, considering both numerical simulations and the statistical elaboration of the results has required a total of more than 5000 core hours and the processing of more than 2TB of data, an effort that wouldn't have been possible without the access to high level HPC resources.

GALES: a general-purpose multi-physics FEM code

Deepak Garg, Paolo Papale, Antonella Longo, and Chiara Montagna

National institute of Geophysics and Volcanology, Pisa, Italy

We present a versatile open-source FEM-based multi-physics numerical code GALES for volcanic and general-purpose problems. The code is developed/applied to a suite of problems in magma and volcano dynamics.

The software is written in modern C++ and is parallelized using OpenMPI and Trilinos libraries. GALES comprises several advanced solvers for 2D and 3D problems dealing with heat transfer, compressible to incompressible mono and multi-fluid flows in Eulerian and Arbitrary Lagrangian-Eulerian (ALE) formulations, Elastic (static and dynamic) deformation of solids and fluid-solid interaction. Fluid solvers account for both Newtonian and non-Newtonian rheologies. Solvers account for transient as well as steady problems. Non-linear problems are linearized using Newton's method.

All solvers have been thoroughly verified and validated on standard benchmarks. The software is regularly used for high-performance computing (HPC) on our local cluster machines at INGV, Pisa, Italy. Recently, we analyzed the performance of the code by a series of strong-scaling tests conducted on the Marenostrum supercomputer at the Barcelona Supercomputing Centre (BSC) up to 12288 cores. The results revealed a computational speedup close to ideal and above satisfactory levels as long as the element/core ratio is sufficiently large, making GALES an excellent choice for utilizing HPC resources efficiently for complex magma flow and rock dynamics problems.

HPC in Rapid Disaster Response: Numerical simulations for hazard assessment of a potential dam breach of the Kyiv cistern reservoir, Ukraine

Carlos Sánchez-Linares, Jorge Macías, and Manuel J. Castro Díaz

EDANYA Group - University of Málaga. Málaga, Spain

In this work, we demonstrate the importance of High Performance Computing (HPC) and Urgent Computing (UC) in rapid disaster response to man-made catastrophes. Using the specific case study of a potential dam breach at the Kyiv cistern reservoir in Ukraine, we show how these technologies can be used to assess the potential hazards and impacts of such an event.

The Copernicus Emergency Management Service Risk & Recovery Mapping service was activated to derive hazard assessment mapping for the protection of citizens and infrastructure in the event of a potential dam breach. The Kiev Hydroelectric Power Plant, located upstream of Kiev, has been the target of a previous rocket attack, and the threat of another successful attack cannot be ruled out. The potential consequences of a dam breach are severe and include flooding and the erosion and transport of radioactive sediment.

To determine the impact of a potential dam breach and predict its effects on citizens and infrastructure, we used the Dambreak-HySEA model, which is part of the HySEA suite. This model is specifically designed to accurately reproduce the evolution of wet/dry fronts in geophysical flows such as river flooding, flooding in rural and urban areas, and dam failures. Developed by the research group EDANYA of the University of Malaga, the model was implemented using Graphics Processor Units (GPUs) with CUDA, resulting in a significant speed-up compared to a traditional CPU implementation.

The use of HPC resources, specifically those provided by the Spanish Network for Supercomputing (RES) program Urgent computing for citizen problems, was crucial in obtaining the results within the 10-day delivery time frame with the simulation of four scenarios required by the activation: partial and complete breakage of the Kyiv Dam and the same scenarios for the Irpin Dam. These simulations were computationally complex, requiring the solution of nearly 700 million computational cells per scenario.

Overall, this study highlights the importance of utilizing HPC and UC in disaster response and risk management. By utilizing advanced numerical models and computational resources, we can more accurately predict the potential hazards and impacts of man-made catastrophes such as dam breaches, and take necessary measures to protect citizens and infrastructure.

Physics-informed Neural Networks to Simulate Subsurface Fluid Flow in Fractured Media

Linus Walter[1,2,3], Francesco Parisio[4], Qingkai Kong[5],
Sara Hanson-Hedgecock[3], and Víctor Vilarrasa[3]

[1]Institute of Environmental Assessment and Water Research (IDAEA), Spanish National Research Council (CSIC), Barcelona, Spain, [2]Associated Unit: Hydrogeology Group (UPC-CSIC), Barcelona, Spain, [3]Global Change Research Group (GCRG), Mediterranean Institute for Advanced Studies (IMEDEA), CSIC-UIB, Esporles, Spain, [4] Independent, [5]Lawrence Livermore National Laboratory, Livermore, USA

Reliable reservoir characterization of the strata, fractures, and hydraulic properties is needed to determine the energy storage capacity of geothermal systems. We apply the state-of-the-art Physics-Informed Neural Networks (PINN) to model subsurface flow in a geothermal reservoir. A PINN can incorporate any physical laws that can be described by partial differential equations.

We obtain a ground truth dataset by running a virtual pumping-well test in the numerical code “Code_Bright”. This model consists of a low-permeability rock matrix, intersected by high-permeability fractures. We approximate the reservoir permeability with an Artificial Neural Network (ANN) denoted by . Secondly, we model the fluid pressure evolution with the PINN by informing it about the experimental well-testing data. Since observation wells are sparse in space (only the injection well in our case), we feed into a hydraulic mass balance equation. The residual of this equation enforces the loss function of for random collocation points inside the domain.

Our results indicate that the ANN is able to approximate even for a high permeability contrast. In addition, the successful interpolation of proves the PINN is a promising method for matching field data with physical laws. In contrast to numerical models PINNs shift the computational efforts toward the training, while reducing the resources needed for the forward evaluation. Nevertheless, training a 3D reservoir model can hardly be achieved on an ordinary workstation since the training data may include several millions of entries. In addition, computational costs increase due to the inclusion of multiphysics processes in the PINN. We plan to prepare the PINN model for training using parallelized GPUs to significantly increase the training speed of the ANNs.

Coupled permafrost-groundwater simulation applied to a spent fuel nuclear waste repository

Thomas Zwinger[1], Denis Cohen[2,3], and Lasse Koskinen[4]

[1]CSC - IT Center for Science Ltd., High Performance Computing, Espoo, Finland, [2] New Mexico Tech, Socorro, NM, United States of America, [3] CoSci LLC, Orlando, FL, United States of America, [4] Posiva Oy Olkiluoto, Eurajoki, Finland

The Olkiluoto spent nuclear fuel repository in Eurajoki, Finland, is the first one on the planet that will go operational in foreseeable future. The long-term safety of this repository with respect to future ice-age conditions and the consequently occurring permafrost and altered groundwater flow conditions needs to be evaluated. To this end, a Darcy model for saturated aquifer groundwater flow combined with a heat transfer module accounting for phase change (i.e. freezing) as well as a solute and a bedrock deformation model have been implemented in the multi-physics Finite Element Method code Elmer.

The set of equations is based on continuum thermo-mechanic principles. The application of this newly developed model to Olkiluoto aims to simulate the evolution of permafrost thickness, talik development, and groundwater flow and salinity changes at and around the repository during the next 120,000 years. This is achieved by solving the aforementioned model components in a coupled way in three dimensions on the mesh that discretizes a rectangular block of 8.8 km by 6.8 km, stretching from the surface of Olkiluoto down to a depth of 10 km, where a geothermal heat flux is applied. The horizontal resolution of 30 m by 30 m in combination with – imposed by the thickness of different temporarily varying soil and rock layers imported from high resolution data - vertical resolutions of down to 10 cm result in a mesh containing 5 million nodes/elements on which the system of equations is solved using CSC's HPC cluster mahti. The high spacial gradients in permeability (e.g. from soil to granitic bedrock) impose numerical challenges for the simulations that are forced by RCP 4.5 climate scenario. The investigated time-span contains cold periods between AD 47,000 and AD 110,000. Surface conditions are provided using freezing/thawing n-factors based on monthly temperature variations and wetness index defining varying conditions of vegetation. Our scenario run is able to project permafrost development at high spatial resolution and shows clear impact of permeable soil layers and faults in the bedrock that focus groundwater flow and solute transport.

Risk assessment and mitigation of induced seismicity for geo-energy related applications at the basin scale

Haiqing Wu[1,2], Jian Xie[3], and Victor Vilarrasa[4]

[1] Department of Civil and Environmental Engineering (DECA), Universitat Politécnica de Catalunya (UPC), Barcelona, Spain [2] Associated Unit: Hydrogeology Group (UPC-CSIC), Barcelona, Spain, [3] College of Environment and Civil Engineering, Chengdu University of Technology, Chengdu, 610059, China, 4 Global Change Research Group (GCRG), IMEDEA, CSIC-UIB, Spain

Fluid injection-induced earthquakes involve a series of complex physical processes. Evaluating these processes at the basin scale requires an amount of input data and a super computational ability to solve in near-real time risk analysis, which remains the most critical challenge in geo-energy related applications. Although the current computational tools can achieve a good simulation for the field scale problems, they are far away from the requirements of the basin scale analysis. Alternatively, we can apply verified analytical solutions of certain processes to speed the whole calculations when moving from the field to the basin scale. With this in mind, we adopt the analytical solutions for pore pressure diffusion and stress variations due to fluid injection into the reservoir. With the superposition principle, the analytical solutions can address the coupling problem of multi-injection wells at the basin scale. We then assess faults stability and the associated induced seismicity potential using the hydro-mechanical perturbations throughout the basin computed analytically.

To handle the uncertainty of geological properties, including the fault and reservoir geometries, hydraulic and mechanical properties, we perform Monte Carlo simulations to analyze their effects on induced seismicity potential. Such comprehensive parametric space analysis currently represents an insurmountable obstacle to be solved numerically, even calculating the problem in parallel. We propose a feasible methodology to mitigate the magnitude of induced seismicity, and even to avoid large earthquakes for subsurface energy-related projects, based on the results obtained both at the field and basin scales. This development will represent a great tool for risk evaluation of induced earthquakes not only in the period of site selection, but also in the whole lifetime of geo-energy projects.

Optimal source selection for local probabilistic tsunami hazard analysis

Alice Abbate[1,2], Manuela Volpe[1], Fabrizio Romano[1], Roberto Tonini[1], Gareth Davies[3], Roberto Basili[1], and Stefano Lorito[1]

[1]Istituto Nazionale di Geofisica e Vulcanologia, Italy, [2]Department of Mathematics and Geosciences, University of Trieste, Italy, [3]Place, Space and Communities Division, Geoscience Australia, Australia

Local hazard models for evacuation planning should accurately describe the probability of exceeding a certain intensity (e.g. flow depth, current velocity, etc.) over a period of years.

Computational-based probabilistic forecasting for earthquake-generated tsunamis deals with tens of thousands to millions of scenarios to be simulated over very large domains and with sufficient spatial resolution of the bathymetry model. The associated high computational cost can be tackled by means of workflows that take advantage of HPC facilities and numerical models specifically designed for multi-GPU architectures.

For the sake of feasibility, Seismic Probabilistic Tsunami Hazard Assessment (S-PTHA) at local scale exploits some approximations in both source and tsunami modeling, but uncertainty quantification is still lacking in the estimates. Here, we propose a possible approach to reduce the computational cost of local-scale S-PTHA, while providing uncertainty quantification.

The algorithm performs an efficient selection of scenarios based on the tsunami impact on a site.

The workflow is thought to take advantage of parallel execution on HPC clusters. Hence, as a first step, the whole ensemble of scenarios is split into a finite number of regions defined by the tectonic regionalization; then the procedure selects the scenarios mainly contributing to the hazard at an offshore point (in front of the target site) and for specific intensity levels. Finally, for each intensity level, the totality of synthetic tsunamigenic earthquakes is optimally sampled with replacement in a Monte Carlo Importance Sampling scheme.

The tsunamis potentially triggered by the selected scenarios are explicitly simulated with the GPU-based Tsunami-HySEA nonlinear shallow water code on high spatial resolution grids (up to 10 m) and subsequently the Monte Carlo errors are finally propagated to the onshore estimates.

This procedure allows for lessening the computational cost of local S-PTHA by reducing the number of simulations to be conducted while quantifying the epistemic uncertainties associated with the inundation modeling without appreciable losses of information content.

Tsunami evacuation using an agent-based model in Chile

Natalia Zamora[1], Jorge León[2,4], Alejandra Gubler[3,4], and Patricio Catalán[2,4]

[1]Barcelona Supercomputing Center, Barcelona, Spain, [2] Universidad Técnica Federico Santa María, Valparaíso, Chile, [3] Pontificia Universidad Católica de Chile, Santiago, Chile, [4] Centro de Investigación para la Gestión Integrada del Riesgo de Desastres, Chile

Tsunami evacuation planning can be crucial to mitigate the impact on lives. During evacuation procedures, vertical evacuation can be an effective way to provide protection to people if horizontal evacuation is not feasible.

However, this can imply an associated risk if the different scenarios related not only to the uncertainties of the tsunami phenomena, but also to the behavior of people during an evacuation phase are not considered.

For this reason, in recent years, tsunami risk management in Chile has incorporated the propagation of uncertainties in each phase of the study of tsunami impacts and the design of evacuation routes. Agent-based models allow coupling inundation tsunami scenarios and the people's interactions and decision-making. In this research, thousands of tsunami scenarios are considered to establish tsunami hazard mapping based on flow depths and tsunami time arrivals. We chose a worst-case scenario from this database and coupled it with an agent-based model to assess tsunami evacuation in Viña del Mar, Chile.

Moreover, we examined an improved situation with the same characteristics, but including 11 tsunami vertical-evacuation (TVE) facilities. Our findings show that the tsunami flood might lead to significant human casualties in the case of a worst-case scenario (above 50% of the agents). Nevertheless, including the TVE structures could reduce this number by roughly 10%. Future work will include propagation of uncertainties also in all the phases of the evacuation where HPC will aid on the simulations of agent-based models that require intense computational resources.

Exhaustive High-Performance Computing utilization in the estimation of the economic impact of tsunamis on Spanish coastlines

Alejandro Gonzalez del Pino[1], Marta Fernández[3], Miguel Llorente[2], Jorge Macías[1], Julián García-Mayordomo[2], and Carlos Paredes[3]

[1] University of Málaga, Dpto. Análisis Matemático e Investigación Operativa, Spain, 2 Geological Survey of Spain (CN-IGME CSIC), Department of Research and Prospective Geoscience, 3 Departamento de Ingeniería Geológica y Minera, Escuela de Minas y Energía, Universidad Politécnica de Madrid

Tsunamis are low-probability phenomena with high-risk potential. Lack of field data emphasizes the need of using simulation software to model the potential devastating effects of a tsunami and use this information to develop safety, sustainable actions and social resilience for the future. These measures may include, among many others, spatial planning; designing of evacuation routes; or the allocation of economic resources through insurance or other instruments to mitigate tsunami impacts. Our work introduces a Monte Carlo-like method for simulating the potential impact of tsunamis on the Spanish coastlines, specifically in the provinces of Huelva and Cádiz for the Atlantic region, and Balearic Islands, Ceuta, Melilla and eastern Iberian coast for the Mediterranean region.

The method introduces a pseudo-probabilistic seismic-triggered tsunami simulation approach, by considering a particular selection of active faults with associated probabilistic distributions for some of the source parameters, and a Sobol's sequences-based sampling strategy to generate a synthetic seismic catalogue. All roughly 4000 crafted seismic events are simulated along the areas of interest in high-resolution grids (five meters pixel resolution) using a two-way nested mesh approach, retrieving maximum water height, maximum mass flow and maximum modulus of the velocity at each grid cell. These numerical simulations are computed in a GPU environment, harnessing resources allocated in several high-performance computing (HPC) centres. HPC infrastructures play a crucial role in the computing aspect of the project, as the calculation power required to complete full-fledge high-resolution tsunami simulations in a reasonably time is expensive. The numerical database of retrieved variables generated throughout this study offers an excellent foundation for evaluating various tsunami-related hazards and risks.

The final resulting product focuses on generating frequency distributions for the economic impacts for the Spanish insurance sector (Consorcio de Compensación de Seguros, CCS). The CCS is a public-private entity insuring most natural catastrophic events in Spain. A consistent spatially-distributed economic database regarding insurance building-related values has been constructed and aggregated in conjunction with the numerical tsunami simulations.

The proposed procedure allows to associate an economic impact indicator to each source. Further statistical analysis of the economic impact estimators yields to varied conclusions such as an improved definition of worst-case scenario (effect-based rather than worst-triggered), most and least likely economic impact, highest hazardous fault sources overall and locally and many others.

Numerical simulation of injection-induced seismicity

Victor Vilarrasa1, Haiqing Wu2,3, Iman Vaezi1,3,4, Sri Kalyan Tangirala1, Auregan Boyet1,3,4, Silvia De Simone1, and Iman R. Kivi1,3,4

[1]Barcelona Supercomputing Center, Barcelona, Spain, [2] Universidad Técnica Federico Santa María, Valparaíso, Chile, [3] Pontificia Universidad Católica de Chile, Santiago, Chile, [4] Centro de Investigación para la Gestión Integrada del Riesgo de Desastres, Chile

Geo-energies, such as geothermal energy, geologic carbon storage, and subsurface energy storage, will play a relevant role in reaching carbon neutrality and allowing net-carbon removal towards the midcentury. Geo-energies imply fluid injection into and/or production from the subsurface, which alter the initial effective stress state and may destabilize fractures and faults, thereby inducing seismicity.
Understanding the processes that control induced seismicity is paramount to develop reliable forecasting tools to manage induced earthquakes and keep them below undesired levels.

Accurately modeling the processes that occur during fracture/fault slip leading to induced seismicity is challenging because coupled thermo-hydro-mechanical-chemical (THMC) processes interact with each other:

(1) fluid injection causes pore pressure buildup that changes total stress and deforms the rock, (2) deformation leads to permeability changes that affect pore pressure diffusion, (3) fluids reach the injection formation at a colder temperature than that of the rock, which cools down the vicinity of the well, causing changes in the fluid properties (density, viscosity, enthalpy, heat capacity) and cooling-induced stress reduction, (4) the injected fluids are not in chemical equilibrium with the host rock, leading to geochemical reactions of mineral dissolution/precipitation that may alter rock properties, in particular, the shear strength.

In the framework of GEoREST (www.georest.eu), a Starting Grant from the

European Research Council (ERC), we aim at developing forecasting tools for injection-induced seismicity by developing methodologies to efficiently simulate the coupled THMC processes that occur as a result of fluid injection, which allows us to improve the understanding of the mechanisms that trigger induced seismicity.

To this end, we use the fully coupled finite element method software CODE_BRIGHT, which includes capabilities like friction following the Mohr-Coulomb failure criterion with strain weakening and dilatancy, enabling simulations of fracture/fault reactivation.

Our investigations have already contributed to the understanding of the processes that induced the seismicity at the Enhanced Geothermal System (EGS) at Basel, Switzerland, at the Castor Underground Gas Storage, Spain, and the reservoir-induced seismicity at Nova Ponte, Brazil. To achieve scalability and speed up the calculations to eventually manage induced seismicity in real time, we intend to incorporate efficient state-of-the-art linear solvers, like HYPRE and PETSc, in CODE_BRIGHT.

A digital twin component for volcanic dispersal and fallout

Leonardo Mingari[1], Arnau Folch[1], Alejandra Guerrero[1], Sara Barsotti[2], Talfan Barnie[2], Giovanni Macedonio[3], and Antonio Costa[4]

[1]Geociencias Barcelona (GEO3BCN-CSIC), Barcelona, Spain , Spain, [2] Icelandic Meteorological Office (IMO), Iceland, [3] Istituto Nazionale di Geofisica e Vulcanologia (INGV), Osservatorio Vesuviano, Naples, Italy, [4] Istituto Nazionale di Geofisica e Vulcanologia (INGV), Sezione di Bologna, Bologna, Italy

A Digital Twin Component (DTC) provides users with digital replicas of different components of the Earth system through unified frameworks integrating real-time observations and state-of-the-art numerical models. Scenarios of extreme events for natural hazards can be studied from the genesis to propagation and impacts using a single DTC or multiple coupled DTCs.

The EU DT-GEO project (2022-2025) is implementing a prototype digital twin on geophysical extremes consisting of 12 interrelated Digital Twin Components, intended as self-contained and containerised software entities embedding numerical model codes, management of real-time data streams and data assimilation methodologies. DTCs can be deployed and executed in centralized High Performance Computing (HPC) and cloud computing Research Infrastructures (RIs).

In particular, the DTC-V2 is implementing an ensemble-based automated operational system for deterministic and probabilistic forecast of long-range ash dispersal and local-scale tephra fallout. The system continuously screens different ground-based and satellite-based data sources and a workflow is automatically triggered by a volcanic eruption to stream and pre-process data, its ingestion into the FALL3D dispersal model, a centralized or distributed HPC model execution, and the post-processing step.

The DTCs will provide capability for analyses, forecasts, uncertainty quantification, and "what if" scenarios for natural and anthropogenic hazards, with a long-term ambition towards the Destination Earth mission-like initiative.

Integrating 3D physics-based earthquake simulations to seismic risk assessment: The case of Bogotá, Colombia.

Andrea C. Riaño[1,2], Juan C. Reyes[3], Jacobo Bielak[4], Doriam Restrepo[5], Ricardo Taborda[6], and Luis E. Yamin[7]

1 Universidad de los Andes , Civil and Environmental Engineering, Colombia, 2 Carnegie Mellon University , Civil and Environmental Engineering, USA, 3Universidad de los Andes , Civil and Environmental Engineering, Colombia, 4 Carnegie Mellon University , Civil and Environmental Engineering, USA 5 Universidad EAFIT , Ciencias aplicadas e Ingeniería, Colombia 6 Universidad EAFIT , Ciencias aplicadas e Ingeniería, Colombia, 7 Universidad de los Andes , Civil and Environmental Engineering, Colombia

The basin beneath the greater metropolitan area of Bogotá, Colombia, consists of soft material deposits with shear wave velocity $V_s \leq 400$ m/s that reach depths up to 425 m. Located on a high plateau in the eastern cordillera of the Colombian Andes, this highly populated urban area is subject to significant seismic hazards from local and regional fault systems.

The potential ground motion amplification effects during earthquakes due to the presence of soft soil deposits and the surface and sub-surface topography constitute problems of great importance towards better understanding and estimating the seismic risk of the city.

Given the scarcity of seismic data from large magnitude events, and in an effort to advance modern seismic hazard mapping for the region, this study aimed to develop a physics-based framework to generate synthetic ground records that can help to better understand the basin and other amplification effects during strong earthquake shaking in the region, and then to incorporate these effects into the estimation of seismic risk.

To this end, a set of simulations were first conducted on Hercules, the wave propagation octree-based finite element simulator developed by the

Quake Group at Carnegie Mellon University, to reproduce similar conditions to those observed in Bogotá during past seismic events (e.g., 2008 Quetame Earthquake) and to identify the impacts of hypothetical strong earthquakes scenarios.

Then the results from these simulations were then integrated into a new software package for post-processing and assessing the seismic risk in the Bogotá region for different scenarios selected.

Modeling Depth averaged velocity and Boundary Shear Stress distribution with complex flows

Ebissa Kedir[1], Chandra Ojha[2], and Hari Prasad[3]

1 PhD Research Scholar, Dept. of Civil Engineering, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India. 2 Dept. of Civil Engineering, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India, 3 Dept. of Civil Engineering, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India

In the present study, the depth-averaged velocity and boundary shear stress in non-prismatic compound channels with three different converging floodplain angles ranging from 1.43 to 7.59 have been studied. The analytical solutions were derived by considering acting forces on the channel beds and walls. In the present study, five key parameters, i. e non-dimensional coefficient, secondary flow term, secondary flow coefficient, friction factor, and dimensionless eddy viscosity, were considered and discussed. A new expression for non-dimensional coefficient and integration constants were derived based on the novel boundary conditions.

The model was applied to different data sets of the present experiments and experiments from other sources, respectively, to examine and analyse the influence of floodplain converging angles on depth-averaged velocity and boundary shear stress distributions. The results show that the non-dimensional parameter plays an important in portraying the variation of depth-averaged velocity and boundary shear stress distributions with different floodplain converging angles. Thus, the variation of the non-dimensional coefficient needs attention since it affects the secondary flow term and secondary flow coefficient in both the main channel and floodplains. The analysis shows that the depth-averaged velocities are sensitive to a shear stress-dependent model parameter non-dimensional coefficient, and the analytical solutions are well agreed with experimental data when five parameters are included. It is inferred that the developed model may facilitate the interest of others in complex flow modeling.

SESSION 4 HORIZON EUROPE AND EUROHPC POLICIES

KEYNOTE SPEAKER

The European High Performance Computing Joint Undertaking (EuroHPC JU) – Leading the way in European Supercomputing

Linda Gesenhues

European High Performance Computing Joint Undertaking (EuroHPC JU)

The European High Performance Computing Joint Undertaking (EuroHPC JU) is a joint initiative pooling together the resources of the EU, 32 European countries & private partners, it has the objective of making Europe a world leader in supercomputing.

The EuroHPC JU is procuring and installing supercomputers across Europe. Wherever in Europe they are located, European scientists & users from the public sector and industry can benefit from these supercomputers. Free access is already being provided to European research organisations, with wider access planned for the future.

In parallel, the EuroHPC JU is funding an ambitious R&I programme to develop a full European supercomputing supply chain: from processors and software to applications to be run on these supercomputers & know-how to develop strong European expertise.

INVITED TALKS

Access to MareNostrum5 and other European HPC infrastructures

Oriol Pineda and Sergi Girona

Barcelona Supercomputing Center (BCN-CNS)

The European Union, together with its Member States, are strongly investing in deploying a world-class, complete and diverse HPC infrastructure, through the recently-created European High-Performance Computing Joint Undertaking (EuroHPC). The consortium formed by Spain, Portugal and Turkey is one of the key actors of this initiative, participating together with EuroHPC in the acquisition and operation of MareNostrum5, that will reach a TCO above 200M€ over 5 years.

This system will be accessible through the EuroHPC Extreme Scale calls, as well as the national calls from these three countries. Furthermore, BSC as hosting entity will provide direct user support and open scientific collaborations to research groups interested in using this infrastructure.

LUMI supercomputer for European researchers

Thomas Zwinger, Jussi Heikonen, and Pekka Manninen

CSC-IT Center for Science Ltd

LUMI supercomputer, which is currently #3 on the Top500 list and the most powerful system in Europa, started full production earlier this year. LUMI is jointly funded by EuroHPC JU and a consortium of ten countries led by CSC in Finland.

In this presentation we first discuss the architecture of LUMI from the user's point of view. More precisely, we introduce the various partitions that make LUMI exceptionally versatile and suitable for a wide array of applications and workflows.

To fully harness the computing power of the system, programmers must be able to utilize the AMD MI250X GPUs of the system. Accordingly, we present the available GPU programming models and paradigms together with the performance analysis tools. We will provide information on the particular strategies to apply based on the initial situation of the application the user wants to be ported and deployed on LUMI; e.g. in terms of existing code-base, programming language, problem size, etc..

Finally, we discuss the access and support model: There are various modes and call for access available from both EuroHPC and the consortium countries. The support is handled by the distributed LUMI User Support Team to which all the consortium countries contribute. The consortium also runs a comprehensive training programme.

Leonardo: A Simulator4Earth

Piero Lanucara and Giorgio Amati

CINECA

The European supercomputer Leonardo is one of the three pre-exascale systems announced by EuroHPC Joint Undertaking and will be a significant step forward in raising European research in the field of computational science.

CINECA has a long history in supplying the most powerful supercomputers in the world. The strong partnership with the EuroHPC initiative has led to the realization of the Leonardo project, a significant step forward in raising European research in the field of computational sciences.

Leonardo (ranked 4th in the last Top500 list), hosted and managed by CINECA's new data center located in the Technopole of Bologna, will be fully operational within the summer of this year.

Leonardo will have a strategic role in fostering national and international initiatives with a clear focus on Earth Science, actively supporting relevant projects and activities like the second phase (2023-2026) of the EuroHPC Center of Excellence for Exascale in Solid Earth (ChEESE-2P)1, Geo-INQUIRE2, DT-GEO3 and Destination Earth among the others.

In this talk, the Leonardo systems will be introduced, together with the way how CINECA will actively support the scientific ecosystem with emphasis on the support to the Earth community.

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[2] 2022-2024, GA No 101058518.
[3] 2022-2025, GA No 101058129.

Accelerating Time-To-Science in Geophysical Simulations

Ignacio Sarasua and Filippo Spiga

NVIDIA

Accelerated computing is nowadays, de-facto, accepted as the path forward to deploy large-scale energy-efficient scientific and technical computing (including Exascale).

The positive side effect has been a tremendous opportunity for domain scientists to accelerate the pace of discovery and innovation, as well being capable to quickly respond and adapt to unforeseen natural scenarios by quickly deploy computational tools in support of coordinated mitigation strategies and on-the-ground responses (so called 'urgent computing', work pioneered by the ChEESE Eu Centre of Excellence).

The purpose of this talk is to briefly introduce the NVIDIA platform, hardware and software, showcasing few examples of geophysical applications that have been successfully accelerated using NVIDIA GPU and set the stage for the future in computing which involve classic HPC simulations coupled or argument by AI methods.

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