

## 2022 Report of the C20 Commission on Computational Physics

### Commission Members

Chair	Mei-Yin Chou	Taipei
Vice Chair	Andrew Horsfield	United Kingdom
Secretary	Suklyun Hong	Korea
Member	Regina Maphanga	South Africa
Member	Xiaoqun Wang	China
Member	Anthony Maggs	France
Member	Alfonso Munoz Gonzalez	Spain
Member	Derek Leinweber	Australia
Member	Enzo Marinari	Italy
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Member	Igor Mingalev	Russia
Member	Shinji Tsuneyuki	Japan

### Associate Members

Bismarck Vaz da Costa	Brazil
Joan Adler	Israel
Mathias Troyer	USA

We held the first C20 Commission meeting online on February 7, 2022 to get to know each other and to make plans for the coming years. The activities in 2022 are summarized below.

### XXXIII IUPAP International Conference on Computational Physics CCP2022

CCP2022 is the 33rd in a series of meetings of scientists working in the domain of Computational Physics. The Conference on Computational Physics (CCP) is held every year under the auspices of the C20 Commission for Computational Physics of the International Union of Pure and Applied Physics (IUPAP). The conference includes a broad range of computational scientists with common interests in communicating and engaging with their computation-oriented colleagues to exchange information and develop future collaborations. Due to the COVID-19 pandemic, CCP2022 was held on August 1-4, 2022 and was virtual only. The full program is available on the Conference website: <https://ccp2022.odon.utexas.edu/>.

The Chair of CCP2022 was Professor Renata M. Wentzcovitch (Columbia University, USA), and the other organizers included Jim Chelikowsky (University of Texas at Austin, USA), Feliciano Giustino (University of Texas at Austin, USA), and Ellen Zweibel (University of Wisconsin–Madison, USA). The total number of attendees was 947 from 69 countries, with 86 invited talks. We had 190 women who participated, and 17 of them gave invited talks.

Outstanding work of interest for the broad information content was presented in plenary talks:

Plenary Talk #1. Arun Bansil: *A first-principles description of novel superconductors, topological phases, and ultra-thin films beyond graphene*. This talk presented the latest progress on DFT functionals and applications to complex solids.

Plenary Talk #2. Henry Ferguson: *Observing Galaxy Evolution*. This talk presented the cutting-edge astrophysics enabled by observations by the James Webb Space Telescope.

Plenary Talk #3. Guy Cohen: *Quantum Monte Carlo in the steady state*. This talk presented the latest advances in QMC.

Plenary Talk #4. Priya Vashishta: *Machine learning in condensed matter*. This talk presented applications of billion-atom simulations using machine learning reactive potentials.

Plenary Talk #5. Sauro Succi: *Computational explorations of life in the abyss*. This talk presented simulations of water flow mediating the interaction between living sponges in the deep sea.

Plenary Talk #6. Marie Lopez del Puerto: *Computation in the Physics Curriculum*. This talk presented the accomplishments, plans, and activities of the broad educational program supported by the National Science Foundation to sustain computational physics education at the University level across the US.

Plenary Talk #7. Leticia Cugliandolo: *Giorgio Parisi's scientific portray: Complex Systems and much more*. This talk discussed the life and work of Giorgio Parisi, the recent Physics Nobel Prize winner in theoretical and computational statistical physics.

Plenary Talk #8. Jeroen Tromp: *Advances in seismic full waveform inversion*. This talk presented novel methods to model seismic wave propagation in Earth's interior and produce seismic tomographic models.

### **2022 IUPAP Early Career Scientist Prize in Computational Physics**

The 2022 IUPAP Early Career Scientist Prize in Computational Physics was awarded to Dr. Stephen Carr. The citation reads: "*For pioneering theoretical investigations of the physics of two-dimensional materials, and in particular new insights on the electronic properties of twisted bilayer and multilayer structures.*" Dr. Carr graduated from Columbia University in 2015 and received his Ph.D. in physics from Harvard University in 2020. He now works as a postdoctoral researcher at the Brown Theoretical Physics Center at Brown University. The winner was invited to give a talk at our 33rd Annual Conference on Computational Physics (CCP2022) in August, 2022.

### **Future IUPAP International Conference on Computational Physics**

The XXXIV IUPAP International Conference on Computational Physics CCP2023 will be held in Kobe, Japan. The conference will take place between June and August, but the exact date has not yet been determined.

Respectfully submitted,  
Mei-Yin Chou  
Chair, C20 Commission

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### XXXIV IUPAP International Conference on Computational Physics CCP2023

CCP2023 is the 34th in a series of meetings of scientists working in the domain of Computational Physics. The Conference on Computational Physics (CCP) is held every year under the auspices of the C20 Commission for Computational Physics of the International Union of Pure and Applied Physics (IUPAP). The conference includes a broad range of computational scientists with common interests in communicating and engaging with their computation-oriented colleagues to exchange information and develop future collaborations. CCP2023 was held at Kobe International Conference Center in Kobe, Japan on August 4-8, 2023 in a hybrid way, namely, both on-site and online. The full program is available on the Conference website: <https://ccp2023.jp/>.

The Chair of CCP2023 was Professor Yuko Okamoto from Nagoya University. The total number of attendees was 433 from 28 countries, with 41 invited talks. Outstanding work of interest for broad interest was presented in plenary talks:

Plenary Talk #1. Ali Alavi, *Recent progress with the transcorrelated method: combining real-space concepts with orbital-based quantum chemistry*. This talk presented the latest progress on the transcorrelated method in the quantum chemistry theory.

Plenary Talk #2. Takaharu Otsuka, *Nuclear paradigms superseded after 70+ years thanks to supercomputing on K and FUGAKU*. This talk presented the latest results of simulations in the nuclear theory that were obtained by the World-fastest K and FUGAKU supercomputers.

Plenary Talk #3. Marianna Safronova, *Novel approaches to atomic computations and their applications*. This talk presented the latest results of atomic computations.

Plenary Talk #4. Masaru Shibata, *Multi-messenger astrophysics and numerical relativity*. This talk presented the latest results of multi-messenger astrophysics and their interpretation about gravitational waves.

Plenary Talk #5. Yuji Sugita, *Multi-scale molecular dynamics simulation on protein function in intracellular environments*. This talk presented the results of very large scale simulations of biological molecules, especially in the cellular system.

A C20 Commission meeting also took place during CCP2023 in Kobe with several members joining online. Dr. Yuko Okamoto, Chair of CCP2023 provided a status report of the Conference. Dr. Panos Argyrakis, Chair of CCP2024, provided an update on planning for CCP2024 in Thessaloniki, Greece. There was extensive discussion and a number of suggestions were made for Panos and his team to consider.

### **2023 IUPAP Early Career Scientist Prize in Computational Physics**

The 2023 IUPAP Early Career Scientist Prize in Computational Physics was awarded to Dr. Sinéad M. Griffin. The citation reads: " *For her significant achievements in computational materials physics, expanding our understanding of topological quantum materials and establishing new paradigms for dark matter detection.*" Dr. Griffin is a staff scientist in the Materials Sciences Division and Molecular Foundry at Lawrence Berkeley National Laboratory. Originally from Ireland she obtained a B.A. (mod) honours in Theoretical Physics at Trinity College Dublin, followed by a M.Sc. D.I.C. in Quantum Field Theory from Imperial College London. Her doctorate work was carried out at U.C. Santa Barbara and at the E.T.H. Zürich where she received her Dr. Sc. The winner was invited to give a talk at our 34th Annual Conference on Computational Physics (CCP2023) in August, 2023.

### **Future IUPAP International Conference on Computational Physics**

The XXXV IUPAP International Conference on Computational Physics CCP2024 will be held in Thessaloniki, Greece. The conference will take place between June and August, but the exact date has not yet been determined.

Respectfully submitted,  
Mei-Yin Chou  
Chair, C20 Commission

## 2024 Report of the C20 Commission on Computational Physics

### Commission Members

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Vice Chair	Andrew Horsfield	United Kingdom
Secretary	Suklyun Hong	Korea
Member	Regina Maphanga	South Africa
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### XXXV IUPAP International Conference on Computational Physics CCP2024

The Conference on Computational Physics CCP2024 is the annual Conference in a series of meetings, that are held each year in a different city, treating all aspects of Physics that involve computer calculations, in an effort to explain the behavior of different systems in Physics. The meeting is sponsored by The International Union of Pure and Applied Physics (IUPAP), under the direction of the C20 Committee. CCP2024 took place at Porto Palace Hotel Thessaloniki on July 7-12, 2024. The 2024 meeting brought together scientists from all traditional areas in Physics, but will also extend to the new hot topics, such as Quantum Machine Learning, Neuromorphic Computing, use of AI in large-scale Physics experiments, big data and non-conventional data mining methods with a large variety of applications extending to complex systems, such as financial, and social networks, etc. The meeting provided a very fruitful environment to stimulate collaboration between scientists in different disciplines. A European Commission official from Brussels was invited to give the latest development in funding opportunities for collaborative projects. The Chair of CCP2024 was Professor Panos Argyrakis from Aristotle University. The full program is available on the Conference website: <https://ccp2024.physics.auth.gr/>.

A C20 Commission meeting also took place during CCP2024 at Porto Palace Hotel in Thessaloniki on July 10. Members attending on site were Mei-Yin Chou (Chair), Andrew Horsfield (Vice Chair), Suklyun Hong (Secretary), Anthony Maggs, Regina Maphanga, Gian-Marco Rignanese, and Shinji Tsuneyuki. Members joining remotely were Valentino Cooper, Alfonso Munoz Gonzalez, Xiaoqun Wang, and Adler Joan. Dr. Panos Argyrakis, Chair of CCP2024 provided a status report of the Conference. Dr. Markus Eisenbach presented a proposal for CCP2025 to be held in Knoxville, USA. Dr. Suklyun Hong presented a proposal for CCP2026 to be held in Kora. Both proposals were approved.

### **2024 IUPAP Early Career Scientist Prize in Computational Physics**

The 2024 IUPAP Early Career Scientist Prize in Computational Physics was awarded to Dr. Yang Zhang. The citation reads: "*For his significant and innovative achievements in computational study of topological bands and quantum anomalous Hall states in two-dimensional semiconductors.*" Yang Zhang is an Assistant Professor of Physics at the University of Tennessee, Knoxville. He earned his Bachelor's degree in Physics and Mathematics from Tsinghua University in 2015, followed by a Ph.D. in Physics from the Max Planck Institute Dresden in 2019. He then worked as a postdoc at MIT until 2022. The winner was invited to give a talk at our 35th Annual Conference on Computational Physics (CCP2024) in July, 2024.

### **Future IUPAP International Conference on Computational Physics**

The XXXVI IUPAP International Conference on Computational Physics CCP2025 will be held in Knoxville, Tennessee, USA on August 18-22, 2025. The XXXVII IUPAP International Conference on Computational Physics CCP2026 will be held in Seoul, Korea. The conference will take place between June and August, but the exact date has not yet been determined.

Respectfully submitted,  
Mei-Yin Chou  
Chair, C20 Commission