

# Leogang 2024

|                 |               |  |   |   |
|-----------------|---------------|--|---|---|
| Sunday, 14 Jan  | 19:00         | <b>Welcome Reception and Dinner</b>  |   |   |
| Monday, 15 Jan  | 09:00-12:30   | <b>Working Groups</b>  |   |   |
|                 | 12:30-14:00   | <b>Lunch Break</b>   |   |   |
|                 | 14:00-14:30   | <b>Introduction and Tour de Table</b>  | Peter Coveney and Dieter Kranzlmüller   |   |
|                 | 14:30-16:00   | <b>Session 1</b>   |   | <b>Chair:</b> Peter Coveney   |
|                 |               | 20+10 min  | Shantenu Jha  | AI-coupled-HPC workflows are the new scientific applications                                      |
|                 |               | 20+10 min  | Kerstin Kleese van Damme  | On methods and approaches for safe, secure and trustworthy AI                                     |
|                 | 20+10 min     | Alfons Hoekstra  | Trends in Computational Science, in relation to AI and experiences with 'credible computing'          |   |
|                 | 16:00-16:30   | Coffee Break   |   |   |
|                 | 16:30-18:30   | <b>Session 2</b>   |   | <b>Chair:</b> Shantenu Jha  |
|                 |               | 20+10 min  | Elisabeth Mayer   | Visualization of Human-scale Blood Flow Simulation using Intel® OSPRay Studio on SuperMUC-NG      |
| 20+10 min       |               | Tim Weaving  | Quantum Reality: What it takes to perform successful simulations                                      |   |
| 30+30 min       | Nana Liu      | Analogue quantum simulation of PDEs'   |   |   |
| 19:00           | <b>Dinner</b> |  |   |   |
| Tuesday, 16 Jan | 09:00-12:30   | <b>Working Groups</b>  |   |   |
|                 | 12:30-14:00   | <b>Lunch Break</b>   |   |   |
|                 | 14:00-16:00   | <b>Session 3</b>   |   | <b>Chair:</b> Kerstin Kleese van Damme  |
|                 | 20+10 min     | Hendrik Heinz  | The Present and Future of HPC, Computational, and Data-Driven Materials Selection for Fundamental and |   |
|                 | 20+10 min     | Mathew Carbone   | Data-driven methods for science and spectroscopy  |   |
|                 | 20+10 min     | Krishan Kanhaiya   | Nonbonded Models to simulate FCC Metals, Metal oxides and Metal Hydroxides and their applications     |   |
|                 | 20+10 min     | Xibei Zhang  | Combining AI & Physics-Based Methods to Accelerate Drug Discovery                                     |   |
|                 | 16:00-16:30   | Coffee Break   |   |   |
|                 | 16:30-18:30   | <b>Session 4</b>   |   | <b>Chairman:</b> Andrew Grimshaw  |
|                 |               | 20+10 min  | Alfons Hoekstra   | EU developments in the Virtual Human Twin, about UQ in relation to that, and HPC needs of the VHT |
| 20+10 min       |               | Derek Groen  | The SEAVEA Toolkit for VVUQ-enabled HPC simulations   |   |
| 30+30 min       | Peter Coveney | Uncertainty quantification for high-dimensional parameter spaces: physics-based versus artificial intelligence |   |   |
| 19:00           | <b>Dinner</b> |  |   |   |

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|-------------------|--------------------|---------------------------------------|---------------------|---|
| Wednesday, 17 Jan | 09:00-12:30        | <b>Working Groups</b>                 |                     |   |
|                   | 12:30-14:00        | <b>Lunch Break</b>                    |                     |   |
|                   | 14:00-16:00        | <b>Session 5</b>                      |                     | <b>Chair:</b> Hendrik Heinz   |
|                   |                    | 20+10 min                             | Laura Harbach       | Using Agent-Based Modelling to Identify Effective Coping Mechanisms for Climate-Driven Flooding in Bangladesh |
|                   |                    | 20+10 min                             | Eric Signum         | Empirically calibrating an agent-based model of school choice on household-level register data                |
|                   |                    | 20+10 min                             | Laura Promberger    | CernVM-FS: Efficient software and data distribution in distributed, heterogenous systems                      |
|                   | 20+10 min          |                                       |                     |   |
|                   | 16:00-16:30        | Coffee Break                          |                     |   |
|                   | 16:30-18:30        | <b>Session 6</b>                      |                     | <b>Chair:</b> Derek Groen   |
|                   |                    | 20+10 min                             | Andrew Grimshaw     | Addressing the Insatiable Energy Needs of AI with Renewable Energy  |
|                   |                    | 20+10 min                             | Dieter Kranzlmüller | The Impact of AI on climate and what AI can learn from HPC  |
|                   |                    | 20+10 min                             | Peter Coveney       | On the unreasonable effectiveness of floating point numbers in computational science                          |
| 30 min            | Closing Statements | Peter Coveney and Dieter Kranzlmüller |                     |   |
| 19:00             | <b>Dinner</b>      |                                       |                     |   |
| Thursday, 18 Jan  | 09:00              | <b>Breakfast and Depature</b>         |                     |   |