



# PRACE Course: HPC Code Optimisation Workshop

LRZ | 2 – 4 November 2021



# PRACE Training



LRZ as part of the Gauss Centre for Supercomputing (GCS) belongs to the 14 **PRACE Training Centres** that started in 2012-2017-2020:

- Barcelona Supercomputing Center (Spain)
- CINECA Consorzio Interuniversitario (Italy)
- CSC – IT Center for Science Ltd (Finland)
- EPCC at the University of Edinburgh (UK)
- Gauss Centre for Supercomputing (Germany)
- Maison de la Simulation (France)
- GRNET – Greek Research and Technology Network (Greece)
- ICHEC – Irish Centre for High-End Computing (Ireland)
- IT4I – National Supercomputing Center VSB Technical University of Ostrava (Czech Republic)
- SURFsara (The Netherlands)
- TU Wien – VSC Research Center (Austria)
- University ANTWERPEN – VSC & CÉCI (Belgium)
- University of Ljubljana – HPC Center Slovenia (Slovenia)
- Swedish National Infrastructure for Computing (SNIC) (Sweden)



Univerza v Ljubljani



Irish Centre for High-End Computing



IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER



**Mission:** Serve as **European hubs and key drivers of advanced high-quality training** for researchers working in the computational sciences.

<http://www.training.prace-ri.eu/>

# Lecturers

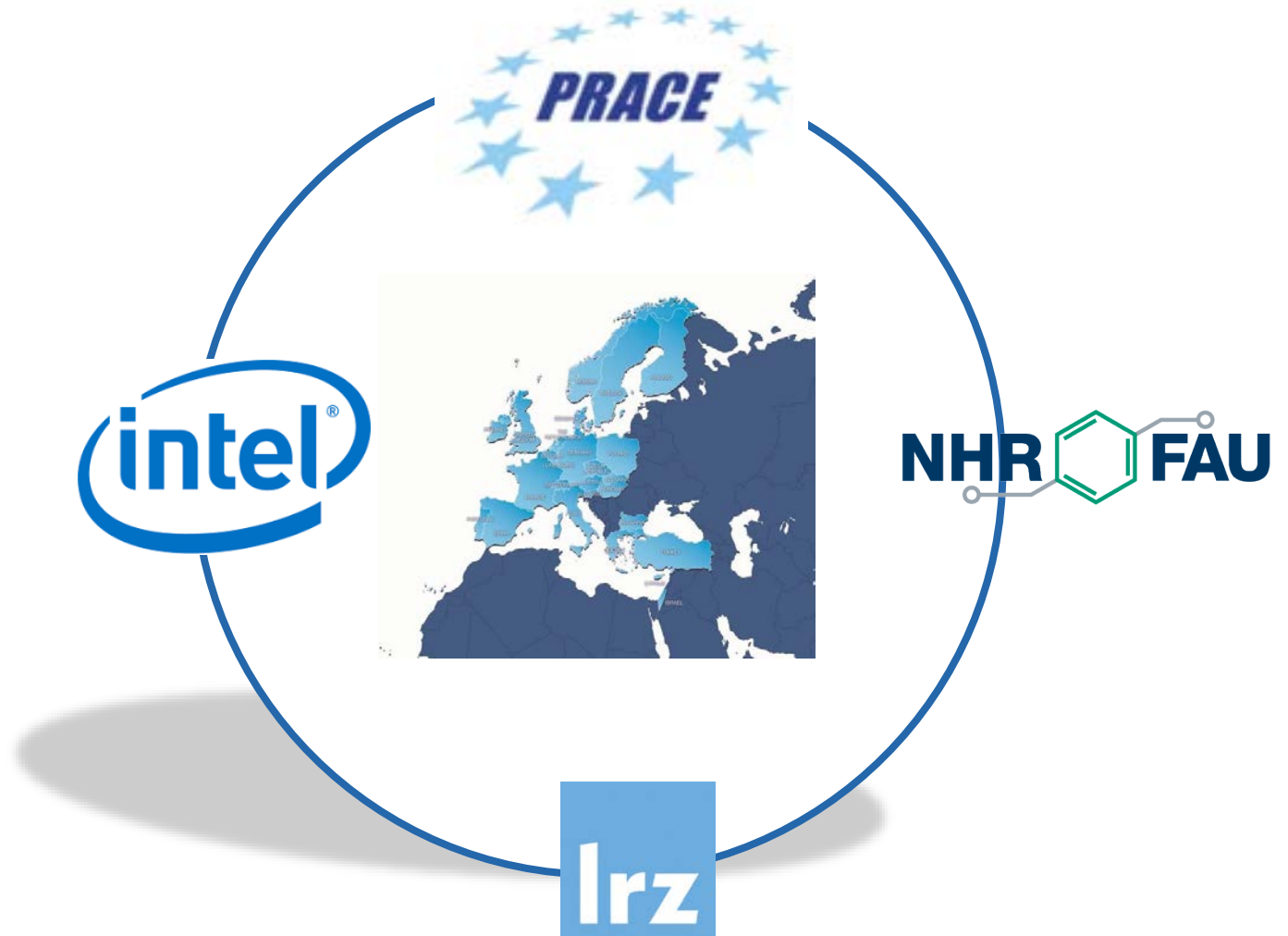


- **Presenters:**

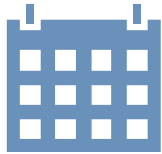
- Jonathan Coles (LRZ)
- Gerald Mathias (LRZ)
- Carla Guillen (LRZ)
- Thomas Gruber (NHR@FAU)
- Edmund Preiss (Intel)
- Alina Shadrina (Intel)
- Michael Steyer (Intel)
- Dmitry Tarakanov (Intel)
- Igor Vorobtsov (Intel)

- **Assistant:**

- Momme Allalen (LRZ)



# Tentative Schedule



	Session
1st day morning (10:00-12:00 CET)	Intro (Volker Weinberg) Intro to LRZ HPC Systems and Software Stack (Gerald Matthias) Intel oneAPI Introduction (Edmund Preiss)
1st day afternoon (13:00-16:00 CET)	Intel Compiler & Vectorization (Igor Vorobtsov /Alina Shadrina)
2nd day morning (10:00-12:00 CET)	Roofline Model (Jonathan Coles) Intel Advisor (Dmitry Tarakanov)
2nd day afternoon (13:00-16:00 CET)	VTune (Michael Steyer) APS (Dmitry Tarakanov) IMPI focus on tuning (Michael Steyer)
3rd day morning (10:00-12:00 CET)	LikWid (Carla Guillen/Thomas Gruber) HPC report (Carla Guillen)
3rd day afternoon (13:00-16:00 CET)	Optimisation highlights by LRZ (CXS Group LRZ)
3rd day Q&A	All

Lectures:

Interleaved with hands-on sessions and short coffee breaks

# Workshop Webpage



- All slides and exercises will be made available under:
- <https://tinyurl.com/code-optimisation-workshop>
  
- Further information on:
  - Agenda
  - Slides
  - Recommended Access Tools
  - How to use the CoolMUC-2 System
  - Intel Software Stack



# How to use the CoolMUC-2 System



- **Login Nodes:**

lxlogin1.lrz.de, lxlogin2.lrz.de, lxlogin3.lrz.de, lxlogin4.lrz.de

Reservation hcow1w21 is only valid during the workshop, for general usage on our Linux Cluster remove the "--reservation=hcowlw21"

- **Submit a job:**

```
sbatch --reservation=hcowlw21 job.sh
```

- **List own jobs:**

```
squeue -M cm2_tiny
```

- **Cancel jobs:**

```
scancel -M cm2_tiny jobid
```

- **Interactive Access:**

```
module load salloc_conf/cm2_tiny
```

```
salloc --partition=cm2_tiny --time=00:30:00 --reservation=hcowlw21
```

```
export OMP_NUM_THREADS=28
```

```
srun --reservation=hcowlw21 ./myprog.exe
```

```
exit
```

```
or: srun --reservation=hcowlw21 --pty bash
```

# Example OpenMP Batch File



```
#!/bin/bash
#SBATCH -o /dss/dsshome1/0B/a2c06ae/test.%j.%N.out
#SBATCH -D /dss/dsshome1/0B/a2c06ae
#SBATCH -J test
#SBATCH --clusters=cm2_tiny
#SBATCH --partition=cm2_tiny
#SBATCH --nodes=1-1
#SBATCH --cpus-per-task=28
#SBATCH --get-user-env
#SBATCH --reservation=hcow1w21
#SBATCH --time=02:00:00

module load slurm_setup
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
./myprog.exe
```

- To ensure a pleasant experience with Zoom Meeting, we encourage participants to **download and install the latest Zoom application** via <https://zoom.us/download>.
- If you have problems with your computer audio, you can also **join by phone**.  
Find your local number: <https://lrz-de.zoom.us/j/aeaPLRITtm>



Zoom Meeting

00:12:30 View

Switch between Speaker View / Gallery View / Fullscreen Mode

Speaker View

✓ Gallery View

Fullscreen

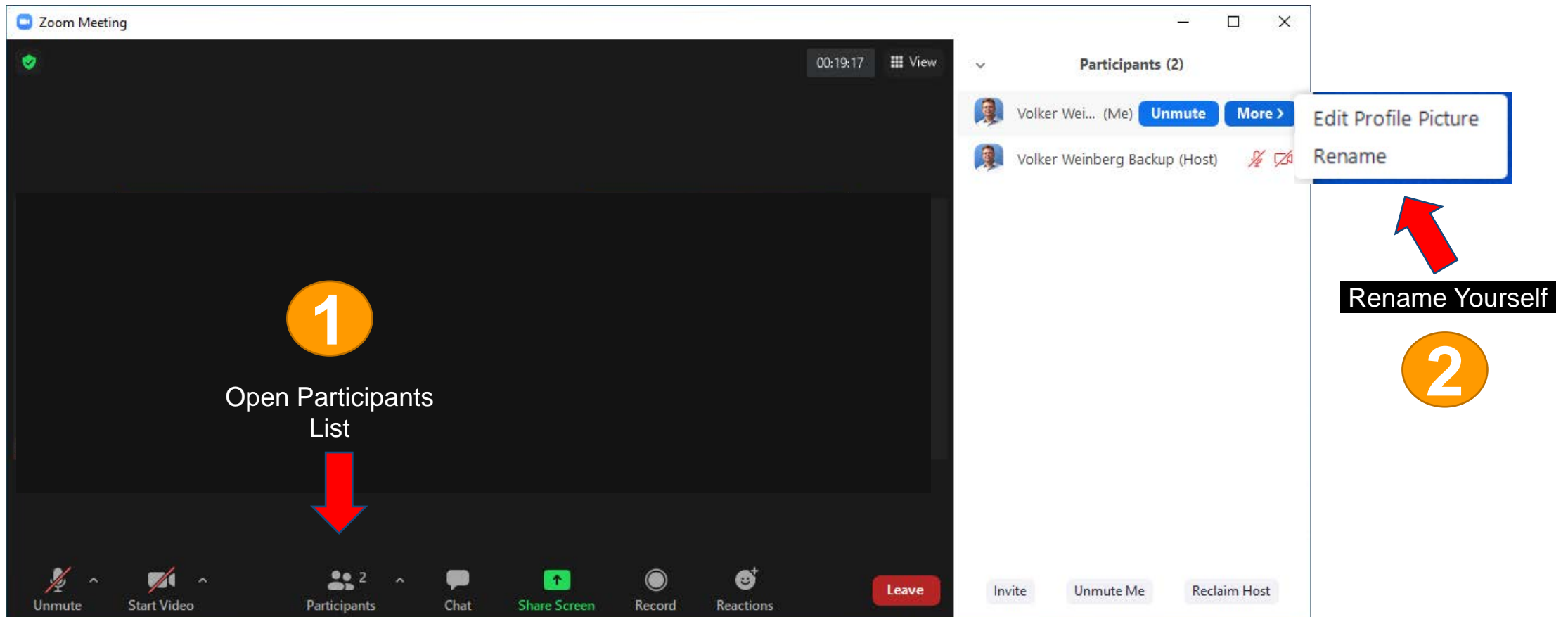
Start / Stop Video / Select Virtual Background

Un-/Mute

Unmute Start Video Participants Chat Share Screen Record Reactions Leave

The screenshot shows the Zoom meeting interface. A red arrow points from the text 'Switch between Speaker View / Gallery View / Fullscreen Mode' to the 'View' dropdown menu, which is open and shows 'Speaker View', 'Gallery View' (selected), and 'Fullscreen'. Another red arrow points from the text 'Start / Stop Video / Select Virtual Background' to the 'Start Video' button in the bottom toolbar. A third red arrow points from the text 'Un-/Mute' to the 'Unmute' button in the bottom toolbar. The bottom toolbar also includes 'Participants', 'Chat', 'Share Screen', 'Record', 'Reactions', and 'Leave' buttons.

Kindly use “first-name family-name (institute)” as your screenname.



The screenshot shows a Zoom Meeting window with a dark background. In the top right corner, the time is 00:19:17 and the view is set to 'View'. The main area is mostly black. At the bottom, there is a toolbar with icons for Unmute, Start Video, Participants (with a '2' next to it), Chat, Share Screen, Record, Reactions, and a red 'Leave' button. A red arrow points from the 'Participants' icon to a white 'Participants (2)' panel on the right. This panel lists two participants: 'Volker Wei... (Me)' and 'Volker Weinberg Backup (Host)'. A blue box highlights the 'More >' button next to the first participant, and a red arrow points to a dropdown menu that contains 'Edit Profile Picture' and 'Rename'. A red arrow also points from the text 'Rename Yourself' to the 'Rename' option. A large orange circle with the number '1' is positioned over the 'Participants' icon in the toolbar, with the text 'Open Participants List' below it. Another large orange circle with the number '2' is positioned below the 'Rename Yourself' text.

1  
Open Participants List

2  
Rename Yourself

Zoom Meeting

00:33:29 View

Chat

Lorem ipsum dolor sit amet.

From Volker Weinberg Ba... to Everyone:

test

From Me to Everyone:

Lorem ipsum dolor sit amet,

Who can see your messages?

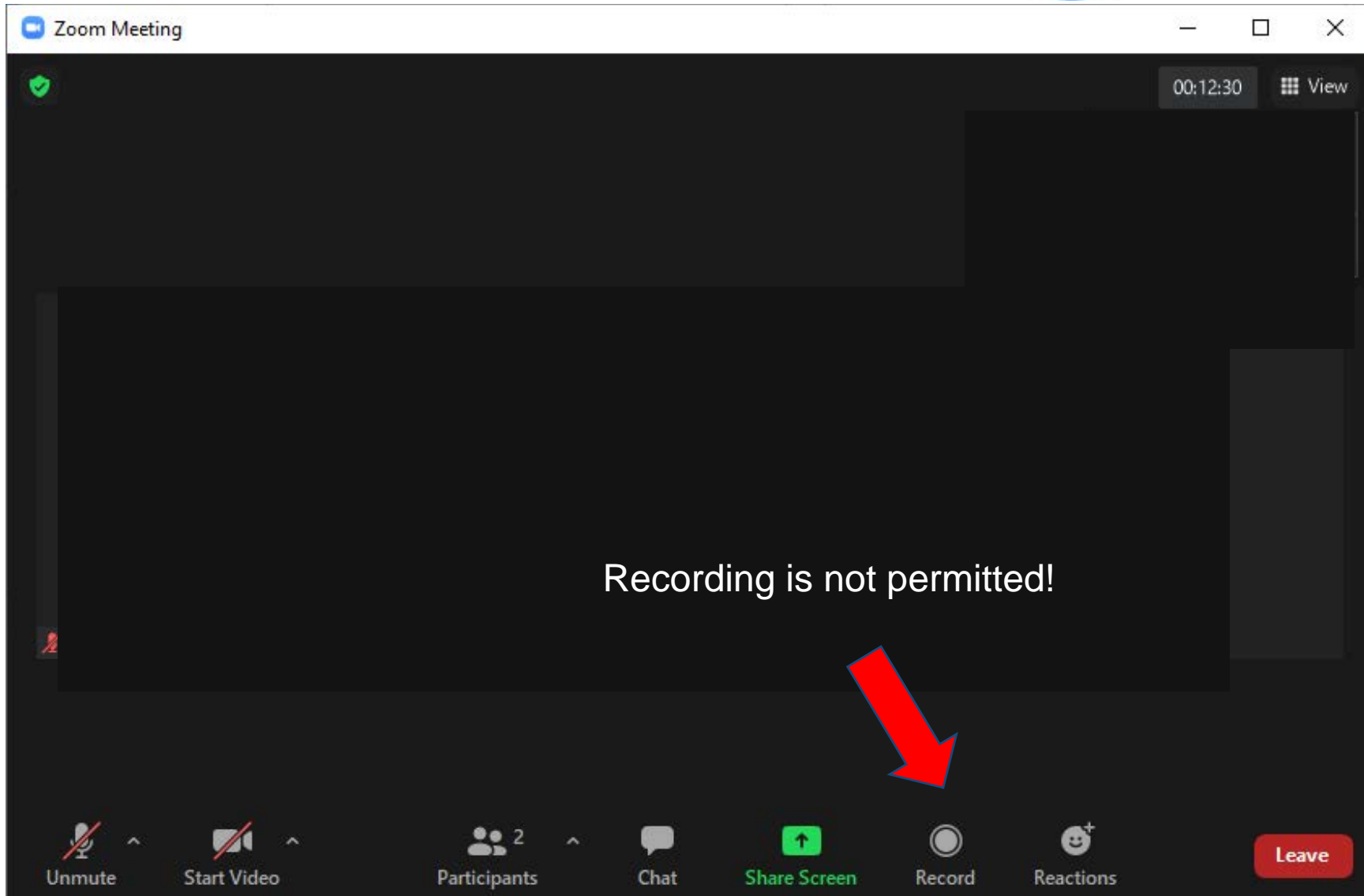
To: Everyone

Type message here...

Unmute Start Video Participants Chat Share Screen Record Reactions Leave

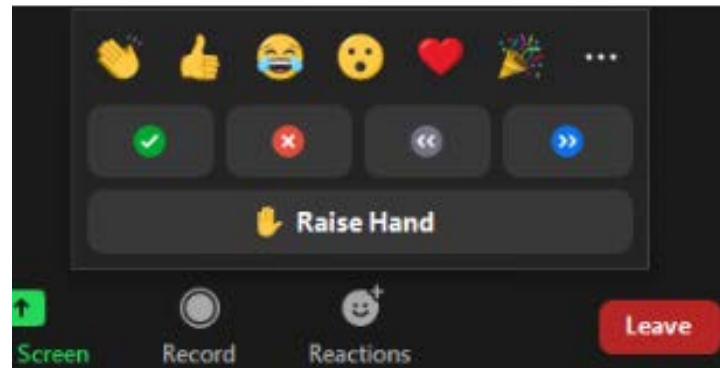
**1**  
Open Chat Window

**2**  
Type Messages Here



- Use **chat window** to ask questions **during the presentations**.
- In **Q&A sessions**:
  - You can also **raise your hand** if you have questions.
  - If you do not mind, please **show your video when asking questions** to make this workshop as interactive as possible.
- **Push to Talk**: The Push to Talk feature allows you to remain muted throughout the Zoom meeting and only if you hold down the spacebar you will be unmuted.

- **Instant Feedback:**



And now ...



**Enjoy the course!**