

DECEMBER 1-2, 2022
SAGRESTIA
SAN FRANCESCO COMPLEX
Lucca

PRO3

joint programme 2022-2023

1st Workshop

**Scientific computing
for natural sciences,
social sciences,
and applications:
methodological
and technological
development**

Here
the link
to follow
the event
in streaming

**THURSDAY,
DECEMBER 1**

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14.25 Greetings and opening address

Marco Paggi (Project coordinator), Scuola IMT Alti Studi Lucca

14.30 Resonance Raman of solvated systems by fully atomistic polarizable QM/MM approaches

Chiara Cappelli, Scuola Normale Superiore

14.55 Modeling Nanoplasmonics: an Atomistic, yet Classical, Approach

Tommaso Giovannini, Scuola Normale Superiore

15.20 Computational Strategies for Environmental Chemistry

Nicola Tasinato, Scuola Normale Superiore

15.45 Coffee break

16.05 Understanding the effect of pathogenic mutations on the structure and function of the voltage-gated potassium channel Kv4.3

Giuseppe Brancato, Scuola Normale Superiore

16.30 A comprehensive characterization of fracture in unit cell open foams generated from Triply Periodic Minimal Surfaces

Pietro Lenarda, Scuola IMT Alti Studi Lucca

16.55 Scientific computing for frontier simulations in tribology

Jacopo Bonari, Scuola IMT Alti Studi Lucca

17.20 Round table

Chiara Cappelli, Scuola Normale Superiore

Gianluigi Rozza, Scuola Internazionale Superiore di Studi Avanzati

Andrea Taramelli, Scuola Universitaria Superiore di Pavia

Nicola Guglielmi, Gran Sasso Science Institute

Marco Paggi, Scuola IMT Alti Studi Lucca

**FRIDAY,
DECEMBER 2**

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- 9.30 Digital twins of the human heart open new routes for cardiovascular research**
Roberto Verzicco, Gran Sasso Science Institute
- 9.55 Retrieval of bio-physical parameters from EO data to develop pre-operational products to improve downstream application services**
Andrea Taramelli and Margherita Righini, Scuola Universitaria Superiore di Pavia
- 10.20 Complexity reduction numerical simulations via general mesh adaptivity**
Andrea Cangiani, Scuola Internazionale Superiore di Studi Avanzati
- 10.55 Coffee break**
- 11.15 Reduced Order Modelling in Computational Mechanics: state of the art and challenges**
Gianluigi Rozza, Scuola Internazionale Superiore di Studi Avanzati
- 11.40 Scientific computing for humanities: artificial intelligence classification of Arabic manuscripts**
Amos Bertolacci and Marco Paggi, Scuola IMT AltI Studi Lucca
- 12.05 Round table**
Chiara Cappelli, Scuola Normale Superiore
Gianluigi Rozza, Scuola Internazionale Superiore di Studi Avanzati
Andrea Taramelli, Scuola Universitaria Superiore di Pavia
Nicola Guglielmi, Gran Sasso Science Institute
Marco Paggi, Scuola IMT AltI Studi Lucca