

High Performance Scientific Computing Using Distributed Infrastructures

Results and Scientific Applications Derived from
the Italian PON ReCaS Project

Giuseppe Andronico • Roberto Bellotti
Guglielmo De Nardo • Giuliano Laccetti
Giorgio Maggi • Leonardo Merola • Guido Russo
Lucia Silvestris • Sabina Tangaro • Enrico Tassi

Editors

High Performance Scientific Computing Using Distributed Infrastructures

**Results and Scientific Applications Derived from
the Italian PON ReCaS Project**

Editors

Giuseppe Andronico

INFN-Catania, Italy

Roberto Bellotti

University of Bari Aldo Moro, Italy

Guglielmo De Nardo

University of Naples Federico II, Italy

Giuliano Laccetti

University of Naples Federico II, Italy

Giorgio Maggi

Polytechnic University of Bari, Italy

Leonardo Merola

University of Naples Federico II, Italy

Guido Russo

University of Naples Federico II, Italy

Lucia Silvestris

INFN-Bari, Italy

Sabina Tangaro

INFN-Bari, Italy

Enrico Tassi

University of Calabria, Italy

 **World Scientific**

NEW JERSEY • LONDON • SINGAPORE • BEIJING • SHANGHAI • HONG KONG • TAIPEI • CHENNAI • TOKYO

Published by

World Scientific Publishing Co. Pte. Ltd.

5 Toh Tuck Link, Singapore 596224

USA office: 27 Warren Street, Suite 401-402, Hackensack, NJ 07601

UK office: 57 Shelton Street, Covent Garden, London WC2H 9HE

Library of Congress Cataloging-in-Publication Data

Names: Laccetti, Giuliano, author. | Programma operativo nazionale ricerca e competitività 2007–2013 (Italy)

Title: High performance scientific computing using distributed infrastructures : results and scientific applications derived from the Italian PON ReCaS Project / Giuliano Laccetti (University of Naples Federico II, Italy), Leonardo Merola (University of Naples Federico II, Italy), Roberto Bellotti (University of Bari Aldo Moro, Italy), Giuseppe Andronico (National Institute for Nuclear Physics (INFN)--Catania, Italy), Guglielmo de Nardo (University of Naples Federico II, Italy), Giorgio Maggi (Polytechnic University of Bari, Italy), Guido Russo (University of Naples Federico II, Italy), Lucia Silvestris (National Institute for Nuclear Physics (INFN)--Bari, Italy), Enrico Tassi (University of Calabria, Italy) & Sabina Tangaro (National Institute for Nuclear Physics (INFN)--Bari, Italy).

Description: New Jersey : World Scientific, 2016. | Includes bibliographical references.

Identifiers: LCCN 2016000016 | ISBN 9789814759700 (hc : alk. paper)

Subjects: LCSH: Science--Italy--Data processing. | Engineering--Italy--Data processing. |

Re.Ca.S. : rete di calcolo per SuperB ed altre applicazioni (Project) |

Re.Ca.S. (Computer network) | Electronic data processing--Distributed processing. |

High performance computing. | Computer networks--Italy.

Classification: LCC Q183.9 .H576 2016 | DDC 502.85/436--dc23

LC record available at <http://lcn.loc.gov/2016000016>

British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library.

Copyright © 2017 by World Scientific Publishing Co. Pte. Ltd.

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the publisher.

For photocopying of material in this volume, please pay a copying fee through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. In this case permission to photocopy is not required from the publisher.

Desk Editors: Kalpana Bharanikumar/Amanda Yun

Typeset by Stallion Press

Email: enquiries@stallionpress.com

Printed in Singapore

Foreword

Started in October 2011 and completed in summer 2015, the ReCaS project was funded by the Italian Ministry of Research and Education (MIUR) through the Italian national *Programma Operativo Nazionale* (National Operational Programme, PON) for “*Research and Competitiveness*” (PON R&C) 2007–2013 Call 254 Action I “*support for structural changes and scientific & technological improvement for a transition towards a knowledge economy*” for the development and enhancement of a distributed computing infrastructure of Grid/Cloud type over the four EU “Convergence” regions in Southern Italy: Campania, Puglia, Sicily, and Calabria.

The acronym ReCaS stands for “*Rete di Calcolo per SuperB e altre applicazioni*” (Computing network for SuperB and other applications). The SuperB was a *Istituto Nazionale Fisica Nucleare* (INFN) project for a new accelerator in the Rome area that has been cancelled by the Italian government due to budget limitations. Now ReCaS is a computing network infrastructure in Southern Italy devoted to scientific and non-scientific applications within the vision of a common European infrastructure for computing, storage, and network.

The actuators are the University of Naples Federico II, the University of Bari Aldo Moro and the Italian National Institute of Nuclear Physics (INFN) with its “sections” in Naples, Bari, Catania, and Cosenza. In Catania and Cosenza sites, there are fundamental operational synergies with the University of Catania and the University of Calabria, respectively.

A lot of experience in the context of previous PON 2000–2006 program, INFN and UE grid projects, has been fully exploited, e.g., SCoPE project in Naples, PI2S2 in Catania.

The main objective of the project is a better integration of the various initiatives already present in Southern Italy, carried out by research and academic institutions, including INFN and Universities. High throughput computing (HTC) and high performance computing (HPC), big data preservation in the medium and long term, need a national infrastructure federated between the various actors in Italy in order to be internationally competitive and integrated in a European Grid/Cloud infrastructure.

As an outcome of the ReCaS project, the present book is published by the World Scientific Publishing and it includes contributions from all the people who used (or collaborate to its maintenance) the ReCaS computing and storage resources for scientific and technological research activities from different scientific domains and applications, e.g., Materials Science and Technology, Aerospace Science and Technology, Mathematics and Computer Science, Chemistry, Life Science, and so on.

All the contributions are organized in different Sections: the first Section collects contributions describing the infrastructure in all its parts (from the hardware description to the policies used for user recruitment and support); the second one collects the contributions which are an overview on the type of applications using the ReCaS infrastructure. Each of the remaining sections collects contributions from a specific scientific/technological domain: Physical Science, Life Science, Engineering, Earth Science, Computer and Computational Science. In the “Physical Science” section there are contributions from the High Energy Physics domain related with the ATLAS, ALICE and The Belle II experiments. In the same section, contributions related with astronomical studies (the KM3Net experiment) and research on non-commutative geometry are also presented. The “Life Science” section includes contributions related to a new approach for the Study of Melanogenesis, the study of the structure of chromosomes in the nucleus of cells and the use of neural network to model complex biological phenomena. In the “Engineering” section are presented contributions from different engineering fields of

interest: the building responses to an earthquake event; the computational simulation of rheology processes; the “in silico” analysis of architectures for the naval and aerospace worlds. In the “Earth Science” section, two contributions are present: the first one discusses results about the numerical simulation of seismic ground motion during the 2009 L’Aquila earthquake, the second one describes the results of the first section related with a new numerical approach for simulation of subsurface hydrological processes. Finally, the “Computer and Computational Science” section collects a first contribution related with a Scalability Analysis of Variational Data Assimilation Algorithms on Hybrid Architectures. All the other contributions in this section are related with the development of tools for the management, monitoring and use of the ReCaS infrastructure resources.

All of the above papers address original research and design and maintenance in the broad field of the HPC systems and environments and several science fields. We collected them with the aim to prepare a volume that could serve as resource for education, information, and reference to professors, researchers, graduate students and the more general HPC community. The editors would like to express their gratitude to the referees for their dedication and expert work in reviewing these papers. Last but not least, we are grateful to all authors for their contributions. We hope that readers will enjoy this volume as much as we enjoyed preparing it.

Leonardo Merola, Roberto Bellotti, Giuseppe Andronico, Guglielmo De Nardo, Giuliano Laccetti, Giorgio Maggi, Guido Russo, Lucia Silvestris, Sabina Tangaro, Enrico Tassi

Naples
September 2016

List of Contributors

M. Alfano

National Institute of Nuclear Physics, Naples, Italy

N. Amoroso

University of Bari A. Moro and National Institute
of Nuclear Physics, Bari, Italy

G. Andronico

National Institute of Nuclear Physics, Catania, Italy

C. Annunziatella

University of Naples Federico II, Naples, Italy

M. Antonacci

National Institute of Nuclear Physics, Bari, Italy

R. Arcucci

Imperial College, London, UK

and University of Naples Federico II and SPACI s.r.l., Naples, Italy

R. Barbera

Università di Catania, Catania, Italy

M. Barbieri

University of Naples Federico II, Naples, Italy

G.B. Barone

University of Naples Federico II, Naples, Italy

E. Begovic

University of Naples Federico II, Naples, Italy

R. Bellotti

National Institute of Nuclear Physics
and University of Bari A. Moro, Bari, Italy

P. Belluomo

National Institute of Nuclear Physics, Catania, Italy

S. Bianco

University of Naples Federico II, Naples, Italy

V. Boccia

National Institute of Nuclear Physics, Naples, Italy

D. Bottalico

University of Naples Federico II, Naples, Italy

C. Bozza

University of Salerno, Salerno and National Institute of Nuclear
Physics, Naples, Italy

A. Brasiello

University of Salerno, Fisciano, Italy

R. Bruno

National Institute of Nuclear Physics, Catania, Italy

F. Cafagna

National Institute of Nuclear Physics, Bari, Italy

G. Calise

University of Naples Federico II, Naples, Italy

R. Campagna

University of Naples Federico II
and National Institute of Nuclear Physics, Naples, Italy

G. Carlino

National Institute of Nuclear Physics, Naples, Italy

- L. Carracciuolo
National Research Council (CNR), Naples, Italy
- P. Castellano
National Institute of Nuclear Physics, Naples, Italy
- M. Castellano
Politecnico of Bari and Genesis Consulting s.r.l, Bari, Italy
- R. Cevenini
National Institute of Nuclear Physics, Naples, Italy
- A.M. Chiariello
University of Naples Federico II, Naples, Italy
- D. Ciliberti
University of Naples Federico II, Naples, Italy
- D.P. Coiro
University of Naples Federico II, Naples, Italy
- F. Colamaria
University of Bari A. Moro
and National Institute of Nuclear Physics, Bari, Italy
- D. Colella
University of Bari A. Moro
and National Institute of Nuclear Physics, Bari, Italy
- S. Corcione
University of Naples Federico II, Naples, Italy
- N. Corriero
Politecnico of Bari, Bari, Italy
- O. Crescenzi
University of Naples Federico II, Naples, Italy
- F. Cristaudo
National Institute of Nuclear Physics, Catania, Italy
- S. Cuomo
University of Naples Federico II, Naples, Italy

- L. D'Amore
University of Naples Federico II,
Naples and Euro Mediterranean Center on Climate Changes (CMCC),
Lecce, Italy
- G. D'Avino
University of Naples Federico II, Naples, Italy
- A. d'Onofrio
University of Naples Federico II, Naples, Italy
- A.H. Day
University of Strathclyde, Glasgow, UK
- M. de Palma
National Institute of Nuclear Physics
and University of Bari A. Moro, Bari, Italy
- G. De Nardo
University of Naples Federico II
and National Institute of Nuclear Physics, Naples, Italy
- P. De Michele
University of Naples Federico II, Naples, Italy
- G. De Monaco
University of Naples Federico II, Naples, Italy
- M. De Corato
University of Naples Federico II, Naples, Italy
- A. De Marco
University of Naples Federico II, Naples, Italy
- F. De Luca
University of Naples Federico II, Naples, Italy
- D. Del Prete
National Institute of Nuclear Physics, Naples, Italy
- S. del Gaudio
University of Naples Federico II, Naples, Italy

- T. Del Vino
Genesis Consulting s.r.l, Bari, Italy
- P. Della Vecchia
University of Naples Federico II, Naples, Italy
- D. Diacono
National Institute of Nuclear Physics, Bari, Italy
- G. Donvito
National Institute of Nuclear Physics, Bari, Italy
- A. Doria
National Institute of Nuclear Physics, Naples, Italy
- D. Elia
National Institute of Nuclear Physics, Bari, Italy
- R. Errico
University of Bari A. Moro, Bari, Italy
- R. Esposito
National Institute of Nuclear Physics, Naples, Italy
- L. Evangelista
National Research Council (CNR), Naples, Italy
- M. Fargetta
National Institute of Nuclear Physics, Catania, Italy
- G. Festa
University of Naples Federico II, Naples, Italy
- A. Franco
National Institute of Nuclear Physics, Bari, Italy
- M. Gaetani d'Aragona
University of Naples Federico II, Naples, Italy
- A. Galletti
University of Naples Parthenope, Naples, Italy
- R. Gervasoni
National Institute of Nuclear Physics, Bari, Italy

F. Giannuzzi

University of Bari A. Moro, Bari, Italy

E. Giorgi

National Institute of Nuclear Physics, Catania, Italy

F. Greco

National Research Council (CNR), Naples, Italy

N. Guarracino

University of Calabria and National Institute of Nuclear Physics,
Arcavacata di Rende, Italy

P. Guida

National Institute of Nuclear Physics, Naples, Italy

G. Ianniruberto

University of Naples Federico II, Naples, Italy

I. Iervolino

University of Naples Federico II, Naples, Italy

A. Incecik

University of Strathclyde, Glasgow, UK

A. Italiano

National Institute of Nuclear Physics, Bari, Italy

G. La Rocca

National Institute of Nuclear Physics, Catania, Italy

G. Laccetti

University of Naples Federico II
and National Institute of Nuclear Physics, Naples, Italy

M. Lapegna

University of Naples Federico II, Naples, Italy

V. Lavorini

National Institute of Nuclear Physics,
Arcavacata di Rende, Italy

F. Lizzi

National Institute of Nuclear Physics
and University of Naples Federico II, Naples, Italy

P.L. Maffettone

University of Naples Federico II, Naples, Italy

G. Maggi

National Institute of Nuclear Physics,
University of Bari A. Moro and Politecnico of Bari, Italy

S. Mancini

University of Naples Federico II, Naples, Italy

G. Manfredi

University of Naples Federico II, Naples, Italy

G. Marrucci

University of Naples Federico II, Naples, Italy

B. Mele

University of Naples Federico II, Naples, Italy

L. Merola

University of Naples Federico II
and National Institute of Nuclear Physics, Naples, Italy

D. Michelino

National Institute of Nuclear Physics, Naples, Italy

P. Migliozzi

National Institute of Nuclear Physics, Naples, Italy

G. Miniello

National Institute of Nuclear Physics
and University of Bari A. Moro, Italy

S. Miranda

University of Naples Federico II, Naples, Italy

A. Monaco

National Institute of Nuclear Physics, Bari, Italy

S. Monforte

National Institute of Nuclear Physics, Catania, Italy

A. Murli

Euro Mediterranean Center on Climate Changes (CMCC),
Lecce and SPACI s.r.l., Naples, Italy

S. Naddeo

National Institute of Nuclear Physics
and University of Naples Federico II, Naples, Italy

M. Nicodemi

University of Naples Federico II,
and National Institute of Nuclear Physics, Naples, Italy

F. Nicolosi

University of Naples Federico II, Naples, Italy

S. Nicotri

National Institute of Nuclear Physics, Bari, Italy

P. Notarangelo

National Institute of Nuclear Physics, Bari, Italy

S. Nuzzo

National Institute of Nuclear Physics
and University of Bari A. Moro, Bari, Italy

M. Paone

National Institute of Nuclear Physics, Catania, Italy

S. Pardi

National Institute of Nuclear Physics, Naples, Italy

G. Park

University of Naples Federico II, Naples, Italy

G. Passaro

National Institute of Nuclear Physics, Catania, Italy

C. Pensa

University of Naples Federico II, Naples, Italy

A. Piccolo

University of Naples Federico II, Naples, Italy

G. Platania

National Institute of Nuclear Physics, Catania, Italy

M. Polese

University of Naples Federico II, Naples, Italy

A. Pombo

Max-Delbrück Centre for Molecular Medicine, Berlin, Germany

A. Prota

University of Naples Federico II, Naples, Italy

C. Rocca

National Institute of Nuclear Physics, Catania, Italy

G. Russo

University of Naples Federico II

and National Institute of Nuclear Physics, Naples, Italy

B. Santeramo

National Institute of Nuclear Physics, Bari, Italy

A. Santo

University of Naples Federico II, Naples, Italy

G. Sava

National Institute of Nuclear Physics, Catania, Italy

R. Scognamiglio

University of Naples Federico II, Naples, Italy

G. Scotti

University of Naples Federico II, Naples, Italy

G. Selvaggi

National Institute of Nuclear Physics

and University of Bari A. Moro, Bari, Italy

G. Severino

University of Naples Federico II, Naples, Italy

F. Silvestri

University of Naples Federico II, Naples, Italy

L. Silvestris

National Institute of Nuclear Physics, Bari, Italy

A. Solla

National Institute of Nuclear Physics, Naples, Italy

V. Spinoso

National Institute of Nuclear Physics, Bari, Italy

B. Spisso

National Institute of Nuclear Physics, Naples, Italy

G. Staiano

University of Naples Federico II, Naples, Italy

S. Tangaro

National Institute of Nuclear Physics, Bari, Italy

M.A. Tangaro

Politecnico of Bari, Bari, Italy

A. Tarasio

National Institute of Nuclear Physics, Arcavacata di Rende, Italy

E. Tassi

University of Calabria and National Institute of Nuclear Physics,
Arcavacata di Rende, Italy

A. Tateo

University of Bari A. Moro, Bari, Italy

A. Tebano

National Institute of Nuclear Physics, Naples, Italy

E. Tinelli

University of Bari A. Moro, Bari, Italy

R. Tognaccini

University of Naples Federico II, Naples, Italy

M. Trofa

Center for Advanced Biomaterials for Health Care @CRIB,
Italian Institute of Technology (IIT)
and University of Naples Federico II, Naples, Italy

R. Valentini

National Institute of Nuclear Physics, Bari, Italy

R. Vela

National Institute of Nuclear Physics, Naples, Italy

F. Ventola

University of Bari A. Moro, Bari, Italy

M. Villari

University of Messina, Messina, Italy

M.M. Villone

Center for Advanced Biomaterials for Health Care @CRIB,
Italian Institute of Technology (IIT)
and University of Naples Federico II, Naples, Italy

G. Vito

University of Bari A. Moro and National Institute
of Nuclear Physics, Bari, Italy

G. Zaccaro

Genesis Consulting s.r.l, Bari, Italy