

Bando per Progetti di ricerca - GNCS 2017

Responsabile: Gianluigi Rozza
Professore Associato Analisi Numerica
SISSA, Scuola Internazionale Superiore di Studi Avanzati,
Area Matematica, mathLab, Tel. 040-3787451
e-mail: gianluigi.rozza@sissa.it
Unità INDAM: SISSA Trieste

Titolo del progetto proposto:

(ENG) Advanced numerical methods combined with computational reduction techniques for parameterised PDEs and applications

(ITA) Metodi numerici avanzati combinati con tecniche di riduzione computazionale per PDEs parametrizzate e applicazioni

Numero dei partecipanti: Politecnico di Milano - MOX 2S + 2T ; Pavia 2S+1T; Trento 2S +1T; SISSA 2S+7T (S=personale strutturato, T=assegnisti e dottorandi): Totale 19

Finanziamento richiesto: 9000 Euro

Premessa

La parte scientifica del progetto è scritta in lingua inglese per garantire una proficua interazione con la componente internazionale dei proponenti non strutturati.

1 Introduzione

The objective of this project is to design and analyse innovative numerical methods for the approximation of partial differential equations (PDEs) in computational science and engineering. The increasing complexity of realistic models and the evolution of computational platforms and architectures are challenging the numerical analysis community to develop more efficient, effective, and innovative methods. We share a consolidated expertise on advanced discretisation schemes based on variational approaches, such as h-type finite elements (FEM), isogeometric analysis (IGA), spectral, and boundary elements (BEM). In several applied fields and scenarios a successive resolution of PDEs with different values of control or design variables or different physical/geometric quantities is required, thus demanding high computational efficiency. We plan to study suitable Reduced Order Methods (ROM), such as reduced basis methods (RBM), proper

orthogonal decomposition (POD) and hierarchical model (HiMod) reduction, representing effective strategies to contain the overall computational costs. We expect that our results will open new scenarios, making possible the solution of more complex problems with significantly reduced computational effort. Applications will play a leading role in the project to highlight demonstrative proofs of concept related with methodological advances, as well as software developments, in order to enhance efficient scientific computing on modern platforms/technological devices.

2 Descrizione sintetica del progetto (max 2 pag)

Several phenomena of interest in applied sciences are modelled as coupled systems of parametrized PDEs. Industrial and clinical researches show nowadays a growing demand of efficient computational tools for multi-query and real-time computations for parametrized systems, such as sensitivity analysis of the haemodynamics in patient-specific biomedical devices or shape optimization of structural parts. Relying on classical high-fidelity discretisation methods for each new query is usually unaffordable due to high computational costs, especially in iterative procedures used for optimization, control, uncertainty quantification, general inverse problems. For these reasons, an increasing amount of research has been devoted in the last decade to reduced order methods. These allow us to obtain accurate and reliable results at greatly reduced computational costs thanks to the selection of few basis functions, representing the most relevant features of the phenomena involved, and to an efficient separation of expensive computations (offline) from the inexpensive (online) reduced-order queries. Reduced order methods (ROMs) proposed in this context, are for instance reduced basis (RB), proper orthogonal decomposition (POD) (and their combination: POD in time and RB in parameters, for instance), hierarchical model reduction (HiMOD), and proper generalized decomposition (PGD) methods.

ROM methodology: We aim at consolidating the development of computational reduction techniques for problems described by parametrized mathematical models, governed by partial differential equations (PDEs). Parameters might be both physical (material properties, nondimensional coefficients such as Reynolds number, boundary conditions, forcing terms) and geometric (i.e., quantities which characterize the shape of the domain). The focus of this project concerns scientific computing and modelling, with a special interest in computational mechanics, electromagnetism, optimization, and control. In all these cases, iterative minimization procedures entailing several numerical resolutions of PDEs (each time with different values of control or design variables or different physical/geometric scenarios) are involved, thus requiring high computational efficiency. For this reason, suitable reduced order model (ROM) techniques, such as reduced basis methods (RBM) and hierarchical model reduction (HiMod), provide an effective strategy to contain the overall computational cost. HiMod, for instance, provides surrogate models for problems characterized by an intrinsic directionality, with transverse components relevant locally. The idea of HiMod is to discretize the full model via a combination of a 1D finite element approximation along the leading direction with

a modal expansion for the transverse dynamics. This leads to solving a system of 1D models. Research activities have led to a significant development of ROM for many problems, and to real-life applications in several scenarios. However, to make these techniques more efficient and viable in a more applied and technological context, several methodological issues are still to be investigated and developed. For instance, in order to perform efficient numerical simulations in complex and variable geometric configurations, as required for instance in engineering or medical applications, ROMs need to be coupled with efficient adaptive and/or parameterization techniques. In order to treat complex geometric properties, the recent developments of the Isogeometric Analysis for curves and surfaces, based on B-Spline or NURBS (Non-Uniform Rational B-Spline), can help ROM to become more performing. This guarantees an efficient and highly integrated treatment and processing of geometries developed within CAD systems, as well as the generation of high-quality computational grids, without resorting to any geometric approximation. To make ROM even more efficient, the combination with BEM (Boundary Element Method) is advisable in linear problems instead of the classical finite elements. Another possible tool to save on the computational cost is represented by the employment of anisotropic adaptive meshes, whose elements are automatically tuned in terms of size, shape, and orientation.

ROM implementation: We plan to develop a versatile and automatic software library for the optimal management of the problem parameters, especially the geometric parametrization, and the coupling of this library with the main packages implementing ROMs. The resulting software will comprise an offline optimized module for the generation of the basis functions and of high-quality adapted meshes, possibly anisotropic, and an online module that will be designed to be used also remotely on a variety of platforms (from laptops to tablets, delocalized), including a graphical interface. The new supercomputer installed at SISSA/ICTP, Ulysses, will be also used for the offline part.

ROM applications: We will focus on: optimal control and inverse problems in electromagnetism; integration of high order methods (IGA), lower dimensionality methods (BEM), and reduced order methods for the efficient management of geometries of industrial and medical interest; computational reduction techniques (reduced basis methods, proper orthogonal decomposition and hierarchical model reduction) and possible interplay. We aim at reducing the online (and possibly the offline) computational time in computational mechanics, fluid dynamics and electromagnetism, in order to address more and more complex problems, taking into account also uncertainty scenarios, and a certain versatility. Other possible applications of interest include naval and mechanical engineering (flows around ships), medicine (fluid-structure interaction problems in the cardiovascular system, as well as the electroencephalography inverse problem) and electric engineering (source identification). All these fields reflect a deep know-how of the senior participants of the project.

ROM Objectives: The research project intends to further improve the capabilities

of the reduced order methods in different fields, in order to face more demanding and complex applications arising in industrial, medical and applied sciences contexts. This research will involve human resources from SISSA, University of Trento, Politecnico di Milano-MOX, University of Pavia. We expect this collaboration to be fruitful in the framework of computational electromagnetism and anisotropic mesh adaptation. More in general, we believe that anisotropic mesh adaptation will improve the computational efficiency in any applicative field exhibiting strong directional features. Developments of advanced reduced order methods will be carefully crafted and adapted in several fields where there is a strong need of computational reduction strategies as well as of parametric studies. In the project the developments of ROM for complex problems in the framework of computational fluid-dynamics and fluid-structure interactions will take advantage of the combined and diversified expertise of the participants of the projects: isogeometric analysis, immersed boundary method, fluid-dynamics and fluid-structure interactions.

Our research project is largely of fundamental and methodological nature, hence we expect to contribute to the advance of knowledge in the framework of numerical analysis for the approximation of PDEs. Nevertheless, we expect that our results will provide new insights for the design of numerical schemes in several application areas. The novelties of our research will concern new analysis tools for the adopted methodologies and new software for scientific computing involving problems ranging from academic examples to real life applications in the fields of fluid-dynamics, electromagnetism, structural mechanics, cardiology and in general multiphysics problems in computational science and engineering.

Models and methods developed within the research program will contribute to open new scenarios in the numerical approximation of PDEs, making it possible the solution of more complex problems with significantly reduced computational times (order of seconds). In addition to industry, the techniques developed within this project have a great potential impact in biomedical and biological fields, ensuring the possibility to increase the complexity of the problems to be addressed, for example by including also uncertainty quantification of some parameters of interest. A remarkable strength of the proposed methodology is the possibility to offer a clear separation between computational resources, together with computational stages. Clusters and supercomputers are useful in the offline stage to generate a basis of solutions, by means of repetitive and expensive computations. Less powerful devices, such as laptops but even tablets or smartphones, enable during the online stage to obtain real-time calculations. The development of the proposed methods is complementary to important investigations dealing with high-performance, large scale, parallel computing environments. By easily accessing a database of pre-computed solutions, reduced-order methods make it promptly available both large computing platforms and increasingly complex mathematical models, such as for example in healthcare or shipyard facilities.

3 Attività del progetto (max 1 pag)

L'interazione tra i partecipanti al progetto prevede una decina di missioni con una spesa media di partecipazione pari a 300 Euro (hotel, viaggio, vitto). Si tratta di missioni brevi di coordinamento ricerca e pianificazione strategica tra Pavia, Milano, Trento e Trieste o per eventi di interesse congiunto. Priorità sarà data ai partecipanti non strutturati nella fase di impostazione del loro lavoro di ricerca, atto a creare forti sinergie ed a trasferire conoscenze pregresse e correnti da parte del personale strutturato.

A questa voce si aggiunge poi la proposta di una giornata di studio con seminari e sessioni tecniche da organizzarsi nell'estate/autunno 2017. Questa proposta si basa sul fatto che iniziative analoghe sono state molto proficue in passato per creare sinergie tra le diverse unità e per indirizzare meglio i dottorandi aderenti al progetto. È previsto inoltre un momento specifico da dedicare alla discussione di esperienze acquisite e strategie di sviluppo di software e librerie open-source per il calcolo scientifico.

È prevista inoltre la partecipazione dei giovani a scuole o conferenze internazionali per lo più in Italia, essendo il 2017 un anno ricco di eventi in Italia legati al calcolo scientifico.

4 Partecipanti al progetto

Partecipanti strutturati

1. **Responsabile:** Gianluigi Rozza

Posizione: Professore Associato in Analisi Numerica

Affiliazione: SISSA, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Area Matematica, mathLab

e-mail: gianluigi.rozza@sissa.it

Pubblicazioni:

1. P. Pacciarini, **G. Rozza**. “Stabilized reduced basis method for parametrized advection-diffusion PDEs”. *Comput. Methods Appl. Mech. Engng*, vol. 274, pp. 1–18, 2014 (con acknowledgements a INDAM-GNCS). SCOPUS 2-s2.0-84896764352.
2. D. Forti, **G. Rozza**. “Efficient geometrical parametrisation techniques of interfaces for reduced-order modelling: application to fluid-structure interaction coupling problems”. *Int. J. Comput. Fluid Dyn.*, vol. 28, no. 3-4, pp. 158-169, 2014 (con acknowledgements a INDAM-GNCS). SCOPUS 2-s2.0-84907380367.
3. F. Negri, A. Manzoni, **G. Rozza**. “Reduced basis approximation of parametrized optimal flow control problems for the Stokes equations”. *Comput. Math. Appl.*, vol. 69, no. 4, pp. 319–336, 2015. SCOPUS 2-s2.0-84922925468.
4. I. Martini, **G. Rozza**, B. Haasdonk. “Reduced basis approximation and a-posteriori error estimation for the coupled Stokes-Darcy system”. *Adv. Comput. Math.*, vol. 41, no. 5, pp. 1131–1157, 2015. SCOPUS 2-s2.0-84948713563.

5. J.S. Hesthaven, **G. Rozza**, B. Stamm. “Certified reduced basis methods for parametrized partial differential equations”. Springer Briefs in Mathematics, BCAM SpringerBriefs, Springer, Cham, 2015, ISBN: 978-3-319-22469-5. SCOPUS 2-s2.0-84955406341.
6. L. Iapichino, A. Quarteroni, **G. Rozza**. “Reduced basis method and domain decomposition for elliptic problems in networks and complex parametrized geometries”, Comput. Math. Appl., vol. 71, no. 1, pp. 408–430, 2016 (con acknowledgements a INDAM-GNCS). SCOPUS 2-s2.0-84953897347.

2. Partecipante: Luca Heltai

Posizione: Ricercatore in Analisi Numerica

Affiliazione: SISSA, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Area Matematica, mathLab

e-mail: luca.heltai@sissa.it

Pubblicazioni:

1. W. Bangerth, D. Davydov, T. Heister, **L. Heltai**, G. Kanschat, M. Kronbichler, M. Maier, B. Turcksin, and D. Wells. “The deal.II library, version 8.4.” Journal of Numerical Mathematics, 2016. SCOPUS 2-s2.0-84990975394.
2. M. Maier, M. Bardelloni, and **L. Heltai**. “LinearOperator – a generic, high-level expression syntax for linear algebra”. Computers and Mathematics with Applications, 72(1):1–24, 2016. SCOPUS 2-s2.0-84971300521.
3. N. Rotundo, T.-Y. Kim, W. Jiang, **L. Heltai**, and E. Fried. “Error analysis of a b-spline based finite-element method for modeling wind-driven ocean circulation”. Journal of Scientific Computing, pages 1–30, 2016. SCOPUS 2-s2.0-84963997998.
4. A. Manzoni, F. Salmoiraghi, and **L. Heltai**. “Reduced Basis Isogeometric Methods (RB-IGA) for the real-time simulation of potential flows about parametrized NACA airfoils”. Computer Methods in Applied Mechanics and Engineering, 284:1147–1180, 2015. SCOPUS 2-s2.0-84921048197.
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3. Partecipante: Stefano Micheletti

Posizione: Professore Associato in Analisi Numerica

Affiliazione: MOX, Dipartimento di Matematica, Politecnico di Milano

e-mail: stefano.micheletti@polimi.it

Pubblicazioni:

1. S. Brugiapaglia, F. Nobile, **S. Micheletti**, S. Perotto. “A theoretical study of compressed solving for advection-diffusion-reaction problems”, *Math. Comp.* (To appear http://www.ams.org/cgi-bin/mstrack/accepted_papers/mcom)
 2. A. Fumagalli, L. Pasquale, S. Zonca, **S. Micheletti**. “An upscaling procedure for fractured reservoirs with embedded grids”, *Water Resour. Res.*, vol. 52, no. 8, pp. 6506–6525. SCOPUS: 2-s2.0-84983591594
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 5. M. Artina, M. Fornasier, **S. Micheletti**, S. Perotto. “The benefits of anisotropic mesh adaptation for brittle fractures under plane-strain conditions”. In *New Challenges in Grid Generation and Adaptivity for Scientific Computing*. Series: SEMA SIMAI Springer, vol. 5, Springer Cham, S. Perotto, L. Formaggia Eds., pp. 43–67, 2015. MR3362235
 6. **S. Micheletti**, S. Perotto, F. David. “Model adaptation enriched with an anisotropic mesh spacing for nonlinear equations: application to environmental and CFD problems”, *Numer. Math. Theor. Meth. Appl.*, vol. 6, no. 3, pp. 447–478, 2013. SCOPUS: 2-s2.0-84879385381
4. **Partecipante:** Simona Perotto
Posizione: Professore Associato in Analisi Numerica
Affiliazione: MOX, Dipartimento di Matematica, Politecnico di Milano
e-mail: simona.perotto@polimi.it
Pubblicazioni:
1. F. Dassi, **S. Perotto**, L. Formaggia. “A priori anisotropic mesh adaptation on implicitly defined surfaces”, *SIAM J. Sci. Comput.*, vol. 37, no. 6, pp. A2758–A2782, 2015. SCOPUS: 2-s2.0-84953209456
 2. T. Taddei, **S. Perotto**, A. Quarteroni. “Reduced basis techniques for nonlinear conservation laws”, *M2AN Math. Model. Numer. Anal.*, vol. 49, no. 3, pp. 787–814, 2015. SCOPUS: 2-s2.0-84927779934
 3. B. Esfandiar, G. Porta, **S. Perotto**, A. Guadagnini. “Impact of space-time mesh adaptation on solute transport modeling in porous media”, *Water Resour. Res.*, vol. 51, no. 2, pp. 1315–1332, 2015. SCOPUS: 2-s2.0-84924690127
 4. S. Brugiapaglia, S. Micheletti, **S. Perotto**. “Compressed solving: a numerical approximation technique for elliptic PDEs based on compressed sensing”, *Comput. Math. Appl.*, vol. 70, pp. 1306–1335, 2015. SCOPUS: 2-s2.0-84940462657

5. F. Dassi, B. Ettinger, **S. Perotto**, L.M. Sangalli. “A mesh simplification strategy for a spatial regression analysis over the cortical surface of the brain”, *Appl. Numer. Math.*, vol. 90, pp. 111–131, 2015. SCOPUS: 2-s2.0-84920103048
 6. **S. Perotto**, A. Veneziani. “Coupled model and grid adaptivity in hierarchical reduction of elliptic problems”, *J. Sci. Comput.*, vol. 60, no. 3, pp. 505–536, 2014. SCOPUS: 2-s2.0-84909625087
5. **Partecipante:** Alessandro Reali
Posizione: Professore Associato
Affiliazione: Università degli Studi di Pavia
e-mail: alessandro.reali@unipv.it
Pubblicazioni:
1. L. Heltai, J. Kiendl, A. DeSimone, **A. Reali**. “A natural framework for isogeometric fluid-structure interaction based on BEM-shell coupling”, *Comput. Methods Appl. Mech. Engng.*, doi:10.1016/j.cma.2016.08.008, 2016 (in press). Scopus: TBA
 2. S. Perotto, **A. Reali**, P. Rusconi, A. Veneziani. “HIGAMod: A Hierarchical IsoGeometric Approach for MODel reduction in curved pipes”, *Computers and Fluids*, doi:10.1016/j.compfluid.2016.04.014, 2016 (in press). Scopus: 2-s2.0-84964601044
 3. F. Auricchio, F. Brezzi, A. Lefieux, **A. Reali**. “An “immersed” finite element method based on a locally anisotropic remeshing for the incompressible Stokes problem”, *Comput. Methods Appl. Mech. Engng.*, vol. 294, pp. 428–448, 2015. Scopus: 2-s2.0-84992391283
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 6. **A. Reali**, H. Gomez. “An isogeometric collocation approach for Bernoulli-Euler beams and Kirchhoff plates”, *Comput. Methods Appl. Mech. Engng.*, vol. 284, pp. 623–636, 2015. Scopus: 2-s2.0-84949116110
6. **Partecipante:** Simone Morganti
Posizione: Ricercatore TD (tipo A)
Affiliazione: Università degli Studi di Pavia
e-mail: simone.morganti@unipv.it
Pubblicazioni:

1. D. Gallo, A. Lefieux, **S. Morganti**, A. Veneziani, A. Reali, F. Auricchio, M. Conti, U. Morbiducci. “A Patient-Specific Follow Up Study of the Impact of Thoracic Endovascular Repair (TEVAR) on Aortic Anatomy and on Post-Operative Hemodynamics”, Computers and Fluids, vol. 141, pp. 54-61, 2016. SCOPUS: 2-s2.0-84965046031.
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7. **Partecipante:** Ana Alonso Rodríguez
Posizione: prof. associato in Analisi Numerica
Affiliazione: Università degli Studi di Trento, Dipartimento di Matematica
e-mail: ana.alonso@unitn.it
Pubblicazioni:

1. **A. Alonso Rodríguez**, J. Camaño, R. Ghiloni, A. Valli. “Graphs, spanning trees and divergence-free finite elements in domains of general topology”. IMA J. Numer. Anal. (Published online October 3, 2016; doi:10.1093/imanum/drw047)
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8. **Partecipante:** Alberto Valli
Posizione: prof. ordinario in Analisi Matematica
Affiliazione: Università degli Studi di Trento, Dipartimento di Matematica
e-mail: alberto.valli@unitn.it
Pubblicazioni:
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 3. A. Alonso Rodríguez, **A. Valli**. “Finite element potentials”. Appl. Numer. Math., vol. 95, pp. 2–14, 2015. MR3349682
 4. A. Alonso Rodríguez, E. Bertolazzi, R. Ghiloni, **A. Valli**. “Construction of a finite element basis of the first de Rham cohomology group and numerical solution of 3D magnetostatic problems”. SIAM J. Numer. Anal., vol. 51, no. 4, pp. 2380–2402, 2013. MR3090156

Partecipanti non strutturati

9. **Partecipante:** Francesco Ballarin
Posizione: assegnista progetto PRIN “Modellistica Matematica per il sistema cardiovascolare umano”
Affiliazione: SISSA, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Area Matematica, mathLab
e-mail: francesco.ballarin@sissa.it
Pubblicazioni:
 1. F. Salmoiraghi, **F. Ballarin**, L. Heltai, G. Rozza. “Isogeometric analysis-based reduced order modelling for incompressible linear viscous flows in parametrized shapes”. Adv. Model. Simul. Eng. Sci., vol. 3, no. 1, pp. 1–21, 2016 (con acknowledgements a INDAM-GNCS). SCOPUS: TBA

2. **F. Ballarin**, G. Rozza. “POD–Galerkin monolithic reduced order models for parametrized fluid-structure interaction problems”. *Int. J. Numer. Methods Fluids*, vol. 82, no. 12, pp. 1010–1034, 2016 (con acknowledgements a INDAM-GNCS). Scopus: 2-s2.0-84978264469
3. **F. Ballarin**, E. Faggiano, S. Ippolito, A. Manzoni, A. Quarteroni, G. Rozza, R. Scrofani. “Fast simulations of patient-specific haemodynamics of coronary artery bypass grafts based on a POD–Galerkin method and a vascular shape parametrization”. *J. Comput. Phys.*, vol. 315, pp. 609–628, 2016. Scopus: 2-s2.0-84963568305
4. **F. Ballarin**, A. Manzoni, A. Quarteroni, G. Rozza. “Supremizer stabilization of POD–Galerkin approximation of parametrized steady incompressible Navier-Stokes equations”. *Int. J. Numer. Methods Eng.*, vol. 102, no. 5, pp. 1136–1161, 2015. Scopus: 2-s2.0-84926443273
10. **Partecipante:** Giovanni Stabile
Posizione: assegnista ERC AROMA-CFD
Affiliazione: SISSA, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Area Matematica, mathLab
e-mail: giovanni.stabile@sissa.it
11. **Partecipante:** Marco Tezzele
Posizione: assegnista progetto ottimizzazione con CNR-INSEAN TRIM-OPT (Cluster TRIM)
Affiliazione: SISSA, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Area Matematica, mathLab
e-mail: marco.tezzele@sissa.it
12. **Partecipante:** Federico Pichi
Posizione: dottorando primo anno in Analisi Matematica, Modelli e Applicazioni
Affiliazione: SISSA, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Area Matematica, mathLab
e-mail: federico.pichi@sissa.it
13. **Partecipante:** Saddam Hijazi
Posizione: dottorando primo anno in Analisi Matematica, Modelli e Applicazioni
Affiliazione: SISSA, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Area Matematica, mathLab
e-mail: saddam.hijazi@sissa.it
14. **Partecipante:** Zakia Zainib
Posizione: dottoranda secondo anno in Analisi Matematica, Modelli e Applicazioni

Affiliazione: SISSA, Scuola Internazionale Superiore di Studi Avanzati, Trieste,
Area Matematica, mathLab
e-mail: zakia.zainib@sissa.it

15. **Partecipante:** Shafqat Ali

Posizione: dottorando terzo anno in Analisi Matematica, Modelli e Applicazioni

Affiliazione: SISSA, Scuola Internazionale Superiore di Studi Avanzati, Trieste,
Area Matematica, mathLab

e-mail: shafqat.ali@sissa.it

16. **Partecipante:** Massimo Carraturo

Posizione: dottorando primo anno in Ingegneria Civile e Architettura

Affiliazione: Università degli Studi di Pavia, Dipartimento di Ingegneria Civile
e Architettura

e-mail: massimo.carraturo01@universitadipavia.it

17. **Partecipante:** Nicola Ferro

Posizione: dottorando del secondo anno (XXXI° ciclo) in Modelli e Metodi
Matematici per l'Ingegneria

Affiliazione: Politecnico di Milano

e-mail: nicola.ferro@polimi.it

18. **Partecipante:** Yves Antonio Brandes Costa Barbosa

Posizione: dottorando del primo anno (XXXII° ciclo) in Modelli e Metodi Matem-
atici per l'Ingegneria

Affiliazione: Politecnico di Milano

e-mail: yvesantonio.brandes@polimi.it

19. **Partecipante:** Juan Luis Valerdi Cabrera

Posizione: dottorando terzo anno (XXX° ciclo) in Matematica

Affiliazione: Università degli Studi di Trento, Dipartimento di Matematica

e-mail: juan.valerdicabrera@unitn.it

5 Budget di previsione

L'interazione tra i partecipanti al progetto prevede una decina di missioni con una spesa media di partecipazione prevista pari a 300 Euro (hotel, viaggio, vitto). Si tratta di missioni brevi di coordinamento ricerca e pianificazione strategica tra Pavia, Milano, Trento e Trieste o per eventi di interesse congiunto. Priorità sarà data ai partecipanti non strutturati nella fase di impostazione del loro lavoro di ricerca, atto a creare forti

sinergie ed a trasferire conoscenze pregresse e correnti da parte del personale strutturato. A questa voce si aggiunge poi la proposta di una giornata di studio con seminari e sessioni tecniche da organizzarsi nell'estate/autunno 2017. Questa proposta si basa sul fatto che le giornate precedenti sono state molto proficue per creare sinergie e per l'inquadramento dei giovani, in particolare dei dottorandi aderenti al progetto.

È prevista inoltre la partecipazione dei giovani a scuole o conferenze estive, per esempio IACM FEF (Finite Element for Flows) 2017 organizzata il 5-7 Aprile 2017 a Roma, (<http://congress.cimne.com/FEF2017/frontal/default.asp>), il workshop ECCOMAS a tema: ADMOS (Adaptive Modelling and Simulation) 2017 organizzato il 26-28 giugno 2017 a Verbania (<http://congress.cimne.com/admos2017/frontal/default.asp>), il workshop QUIET (Quantification of Uncertainty: Improving Efficiency and Technology) 2017 organizzato presso la SISSA il 18-21 Luglio 2017 (<https://indico.sissa.it/event/8/>), la conferenza internazionale IGA 2017 Isogeometrical Analysis a Pavia 11-13 settembre 2017 (<http://congress.cimne.com/iga2017/frontal/default.asp>) e la conferenza ECCOMAS Young Investigators al Politecnico di Milano il 13-15 settembre 2017 (<https://www.eko.polimi.it/index.php/YIC2017/conf>).

In Tabella 1 riassumiamo il quadro complessivo previsto per il budget.

| Voce | KEuro | Descrizione |
|-----------------------------|-------|---|
| Missioni | 3.0 | <i>missioni tra le sedi partner partecipanti al progetto e trasferte eventi</i> |
| Scuole Estive Conferenze | 4.0 | <i>partecipazione giovani</i> |
| Giornata di studio | 2.0 | <i>seminari, tavola rotonda, approfondimenti, discussioni</i> |
| Totale | 9.0 | |

Tabella 1: Quadro riassuntivo delle spese del progetto