

Research Projects
(Call identifier: IP-2020-02)

Application Form¹

Project Proposal Full Title

Multiphysics modelling of surface-subsurface water systems

PROJECT PROPOSAL ACRONYM
Multi-Waters

Please abide by the following text formatting constraints: OpenSans or Arial font, minimum font size 10, margins (right and left margins 2.0, bottom margin 1.5), single line spacing.

The Application Form consists of three parts:

- Part A – Applicant ([pages 1 - 3](#))
- Part B – Project Proposal ([pages 4 – 15](#))
- Part C – Research Group
- References

Cover Page:

- Name of the Applicant – prof.dr.sc. Hrvoje Gotovac
- Name of the scientific organization at which the project will be implemented - University of Split, Faculty of Civil Engineering, Architecture and Geodesy
- Full title of the project proposal - Multiphysics modelling of surface-subsurface water systems
- Project duration (in months) – 48 months

¹ Instructions for completing the Application Form can be found in the Guidelines for Applicants to Croatian Science Foundation's Calls in 2020.

Part A – Applicant

Section a: Applicant's track record in the last 5 years (max. 1 page), including:

1. Five publications: papers in peer reviewed scientific journals with the corresponding link to the peer review journal process, book chapters, conference papers, monographs, etc.

1. Luka Malenica, Hrvoje Gotovac, Grgo Kamber, Srdjan Simunovic, Srikanth Allu, Vladimir Divić; Groundwater flow modeling in karst aquifers: Coupling 3D matrix and 1D conduit flow via control volume isogeometric analysis - experimental verification on 3D physical model, *Water*, (2018), 10(12), 1787; <https://doi.org/10.3390/w10121787>.

2. Galešić, Morena; Andričević, Roko; Gotovac, Hrvoje; Srzić, Veljko. Concentration statistics of solute transport for the near field zone of an estuary. // *Advances in water resources*. 94 (2016); 424-440.

3. Fiori, Aldo; Zarlenga, Alberto; Gotovac, Hrvoje; Janković, Igor; Volpi, Elena; Cvetković, Vladimir; Dagan, Gedeon. Advective transport in heterogeneous aquifers: Are proxy models predictive? // *Water resources research*. 51 (2015), 12; 9577-9594.

4. Cvetković, Vladimir; Gotovac, Hrvoje. On the upscaling of chemical transport in fractured rock. // *Water resources research*. 50 (2014), 7; 5797-5816.

5. Kamber, Grgo; Gotovac, Hrvoje; Kozulić, Vedrana; Malenica, Luka; Gotovac, Blaž. Adaptive isogeometric analysis based on truncated hierarchical basis functions// *Book of Abstracts of the 9th International Congress of Croatian Society of Mechanics*, Split, Hrvatska, (2018), str. 103-112.

2. List of projects (please list projects accepted for funding and project proposals submitted to this or other calls in which you are the PI or an associate. Please state the source of funding, role within the project (Principal Investigator/ Team member) requested or received funds, title of the project. Please provide links to the websites of the funded projects

1. „Monitoring Sea-water intrusion in coastal aquifers and Testing pilot projects for its mitigation“, Researcher/Team member, (total 600 000 Euro): 2019-2022, Interreg IPA project.

2. Interreg CBC Hrvatska-Italija: AdSWiM – Management and treatment of urban wastewater to preserve the quality of the Adriatic coastal area, Hr/Upravljanje i pročišćavanje otpadnih voda urbanih sredina za očuvanje kvalitete obalnog područja Jadranskog mora, Researcher/Team member, (2019-2021).

3. Interreg CBC Hrvatska-Italija: NET4mPLASTIC – New technologies for detection micro and macro plastic on coastal region of Adriatic sea, Hr/ Nove tehnologije za detekciju makro i mikro plastike na obalnom području Jadranskog mora, Researcher/Team member, (2019-2021).

3. Previous participation in HRZZ projects (state your role in the project (Principal Investigator/team member), most important publications resulting from this project and most important results)

„Groundwater flow modeling in karst aquifers“, Croatian Foundation of Science, HRZZ, total 958.000,00 HRK; UIP-2013-8103, Project leader.

2 journal publications (Malenica et al., 2018, Kozulic and Gotovac, 2017), 6 conference publications, 1 PhD dissertation (Malenica, 2019).

All project results are presented in PhD Thesis of Malenica (2019). The main result is the karst flow model and its verification to the laboratory controlled conditions designed in 3-D sandbox (Malenica et al., 2018). Additional project result was development of an adaptive multiresolution method based on new hierarchical Fup basis functions and CV-IGA (initial 1-D results are presented in Kamber et al., 2018). In the one-year post-project phase, three papers are currently in the last stage of the peer review process.

4. Guest lectures at international conferences and/or summer schools

Acex-2018, Engineering modelling with spline based numerical methods, Amsterdam, Holland.

5. Other significant academic achievements: organisation of scientific meetings (201? name of the event and your role /type of event/number of participants/country), international awards, editorial board memberships, longer periods of training courses, international peer review, training courses at international institutions, the most significant scientific collaborations (names of collaborators, topics, organisation, city, country; results application)

Editorial board in journal „International Journal of Engineering modelling“, Training in Oak Ridge National Laboratory, two times by one month (2016 and 2017), International peer review in *Water Resources research*, *Advances in Water Resources*, *Water*, *Geologica Croatica*,....

Collaborations with Vladimir Cvetkovic, Aldo Fiori, Gedeon Dagan, Igor Janković, Srdan Šimunović. Erasmus collaboration with Ramiro Neves, University of Lisbon, 2019.

Section b: Applicant's Curriculum Vitae (max. 2 pages, using the following template)**PERSONAL INFORMATION**

First and last name: Hrvoje Gotovac

Researcher Identification Number: 244885

Personal website: <http://gradst.unist.hr/o-fakultetu/adresar-imenik/agenttype/view/propertyid/1804>

EDUCATION

2009- PhD

Name of the institution: Royal Institute of Technology, KTH, Department of Land and Water resources, Stockholm (Sweden)

2005- Master of Science

Name of the institution: Faculty of Civil Engineering, Architecture and Geodesy, University of Split, Split (Croatia)

1999- Bachelor Degree

Name of the institution: Faculty of Civil Engineering, Architecture and Geodesy, University of Split, Split (Croatia)

Employment

2019 – 2020 – Position: Full professor

Name of the institution: Faculty of Civil Engineering, Architecture and Geodesy, University of Split, Split (Croatia)

Previous employments

2000 – 2019 – Position: From PhD student and Assistant to Associate Professor

Name of the institution: Faculty of Civil Engineering, Architecture and Geodesy, University of Split, Split (Croatia)

SUPERVISION OF DOCTORAL STUDENTS AND POSTDOCTORAL RESEARCHERS

2010 – 2020 24 graduate/2 doctoral theses defended/1 number of supervised postdoctoral researchers:

TEACHING ACTIVITIES

2010-2020 – Scientific area: Technical Sciences: Courses: Hydraulic structures, Groundwater flow and transport modelling

Names of the institution: Faculty of Civil Engineering, Architecture and Geodesy, University of Split, Split; Faculty of Geotechnical Engineering, University of Zagreb

INSTITUTIONAL RESPONSIBILITIES (if applicable)

2010-2018 – Vice-Dean for Science

2016-2020- Chair of Hydro-technics Laboratory

MEMBERSHIPS (e.g. scientific committees or associations; evaluation committees, journal editorial boards, etc.; specify the year and name of the institution) (if applicable):

American Geophysical union

European Geophysical union

Croatian Society of mechanics

Member of Editorial Board of „Journal of Engineering Modelling“

MAJOR SCIENTIFIC COLLABORATIONS (if applicable)

Names of collaborators / Topic / Name of the organisation / City / Country:

1. Royal Institute of Technology, Department of Land and Water Resources, KTH, Stockholm, Sweden. (Professor Vladimir Cvetkovic), subsurface flow and transport, PhD, SKB projects, joint papers.
2. Stockholm University, Sweden. (Professor Georgia Destouni), saltwater intrusion in coastal aquifers, FP5 project.
3. Oak Ridge National Laboratory, Tennessee, USA. (Researcher Srđan Šimunović), HRZZ project.

4. Dipartimento di Ingegneria, Universita' di Roma Tre, Rome, Italy. (Professor Aldo Fiori), subsurface flow and transport, joint papers.
5. Department of Civil, Structural and Environmental Engineering, State University of New York at Buffalo, Buffalo, New York, USA. (Professor Igor Janković), subsurface flow and transport, joint paper.
6. Geotehnički fakultet u Varaždinu, Sveučilište u Zagrebu. (Professor Bojan Đurin), expert project cooperation.
7. Građevinski fakultet u Zagrebu, Sveučilište u Zagrebu. (Professor Goran Lončar), expert project cooperation.
8. Građevinski fakultet u Rijeci, Sveučilište u Rijeci. (Professor Vanja Travaš), expert project cooperation.
9. Croatian Waters (Engineer Ivica Jurčević), expert project cooperation, cooperation on HRZZ project
10. CEMEX (Engineer Kajo Ferić), expert project cooperation.

Part B – Project Proposal

Section a. State of the art in the research area (*describe the state of the art in the research area, highlighting the most important publications.*)

Multiphysics refers to problems that couple multiple physical phenomena. Brown et al. (2008) stated that the science future strongly depends on the following statement: “Today’s problems, unlike traditional science and engineering, do not involve physical processes covered by a single traditional discipline of physics or the associated mathematics. Complex systems encountered in virtually all applications of interest involve many distinct physical processes. The issue of coupling models of different events at different scales and governed by different physical laws is largely wide open and represents an enormously challenging area for future research.”

Semantically, a Multiphysics system consists of more than one component governed by its own principle(s) for evolution or equilibrium, typically conservation or constitutive laws (Keyes et al., 2013). A major classification in such systems is whether the coupling occurs in the bulk (e.g., through source terms or constitutive relations that are active in the overlapping domains of the individual components) or whether it occurs over an idealized interface that is lower dimensional or a narrow buffer zone (e.g., through boundary conditions that transmit fluxes, pressures or displacements). Typical examples of bulk-coupled Multiphysics systems with their own extensively developed literature include radiation with hydrodynamics in astrophysics (radiation-hydrodynamics, or “rad-hydro”), electricity and magnetism with hydrodynamics in plasma physics (magnetohydrodynamics), and chemical reaction with transport in combustion or subsurface flows (reactive transport). Beyond these classic Multiphysics systems are many others that share important structural features (Keyes et al., 2013).

Example of Multiphysics is multiscale simulation where the same component is described by more than one formulation, typically with a computationally defined boundary or transition zone between the domains of applicability. We refer, for example, to schemes based on projective integration keep both fine and coarse models simultaneously in the picture and pass between the different “physics” for reasons of computational complexity. Still other systems may have a Multiphysics character by virtue of being multirate or multiresolution. A chemical kinetics model may treat some components as being in equilibrium, idealizing a fast relaxation down to a constraint manifold on which other components vary more slowly. Stretching the semantics of Multiphysics still further, we may distinguish only between different mathematical formulations or even just different discretization’s of what is essentially the same physical model.

Systems of partial differential equations (PDE) of different types (e.g., elliptic-parabolic, elliptic-hyperbolic, or parabolic-hyperbolic) for the same component may be thought of as Multiphysics because each of the classical partial differential equation archetypes represents a different physical phenomenon. Even a single equation with terms of different types represents a Multiphysics model because each term must often be handled through separate discretization or solver methods.

We enumerate these quotidian examples of multiscale, multirate, multilevel, and multimodel problems because they possess similarities to Multiphysics problems. Some typical large-scale PDE-based Multiphysics applications are fluid-structure interaction, fission reactor fuel performance, reactor core modeling, crack propagation, fusion, subsurface science, hydrology, climate, radiation hydrodynamics, geodynamics and magma dynamics, or accelerator design (Keyes et al., 2013).

In this project, we will concentrate to the Multiphysics fluid complex systems where at least one component consists of a fluid phase in porous media. Particularly, we will take into the consideration Multiphysics of surface-subsurface water systems (SSWS).

A blueprint for modeling fully integrated surface, subsurface, and land-surface hydrological processes, originally proposed forty years ago (Freeze and Harlen, 1969), is now becoming a reality. Although truly coupled models have appeared only recently in the literature (e.g., VanderKwaak and League, 2001; Kollet and Maxwell, 2008), a growing library of models and community of modelers now contribute considerably to our understanding of the coupled terrestrial hydrologic and energy cycles. These coupled and integrated hydrologic models are being used on a range of important issues. The models have common features in that they solve some form of the nonlinear diffusion equation (e.g., Richards) for subsurface water flow and some simpler form of the shallow water equations (usually diffusive wave) for surface flow. Additionally, these hydrologic models are being coupled to land-surface energy, biogeochemistry/ecology models and to atmospheric models. Updated numerical and computational technologies have, in part, enabled new approaches for modeling these coupled interactions. While these models all take different numerical, discretization, and coupling approaches, they share the common goal of modeling—rigorously and mathematically—the terrestrial hydrologic and energy cycle as an integrated system. Research addressing these issues encompasses a range of scales and includes a variety of processes. Hydrologic simulation models break into two broad solution categories: a globally implicit formulation and operator-splitting methods. Among the globally implicit hydrologic models, there are two distinct formulations for solution of

surface and subsurface flow: first-order exchange [VanderKwaak and League, 2001] and continuity of pressure [Kollet and Maxwell, 2008]. Integrated hydrologic models solve equations for surface flow (generally the shallow wave equations) and subsurface flow (generally Richards equation) simultaneously [VanderKwaak and League, 2001] and represent both coupling approaches and a range of numerical implementation of solution (finite-element methods and finite difference/finite-volume methods). While not widespread, integrated hydrologic models have been designed to run on large-scale computing infrastructure and, in one case, demonstrate very good weak scaling out to large numbers of processors.

The state of the art of mentioned Multiphysics modelling shows that related surface-subsurface processes require necessity of multiple different physical formulations for different Multiphysics components, carefully designed coupling strategies between Multiphysics components, needs for new advanced numerical techniques, computation of large-scale numerical and/or stochastic simulations with huge number of unknown degrees of freedom (such as pressure, velocity, concentration, temperature, displacement, etc) in spatial and temporal domain, including high parallel computing (HPC) and adaptive multiresolution and/or multiscale efficient methods and algorithms. Particular question is choice and developing of Multiphysics software since historically it has been done separately for different Multiphysics components within its own disciplines. Final question is verification and validation of Multiphysics software due to its complexity and multiple structures, non-existence of analytic or experimental control solutions and extensive requirements of field measurement data (for example in hydrological models precipitation, hydraulic soil parameters, groundwater velocities and pressures, river flow rate and levels, pollution concentrations, etc). In the sequel, we will try to present how these crucial questions have been solved and analyzed under “the state of art” approaches.

Nowadays, surface-subsurface flow and transport processes is described by 1-D surface flow describes flow in channels, rivers or karst deep conduits. 2-D surface flow describes runoff flow over the upper surface of the domain or fracture flow in fractured (karstified) porous medium (de Rooij, 2013). Mathematical model for subsurface flow is described by Richards nonlinear equation which presents unsaturated flow conditions. Mathematical model for surface flow is described by shallow water equations or usually by its simpler version using the nonlinear diffusive wave equation (Malenica, 2019) which can describe laminar and turbulent flow as well as pressurized or free flow. Mass and energy transport in both domains are described by well known advection-dispersion equation (de Rooij, 2013).

Multidomain approaches require coupling of continuum and/or discrete models in space and, for time-dependent problems, in time. This coupling must respect the mathematical formulation of the coupled problem and must account for different spatial meshes and time discretizations used in each domain. For example, surface-subsurface coupled flow problems of 3-D porous matrix and usually 1-D surface flow in open channels, rivers or karst conduits, coupling is often realized by the first-order exchange flux in the form $[q_{ex} = \alpha_{ex}(h_s - h_m)]$ depending on difference between heads in two fluid domains and exchange parameter which is usually constant, obtained from the calibration process and therefore physically meaningful (see our recent results for surface-subsurface flow interactions in karst aquifers, Malenica et al., 2018). Therefore, particular separate discretization is needed in surface and subsurface domain for heads, but also on interface for exchange flux. Putti and Paniconi (2015) presented overall review about modelling in surface-subsurface water systems and especially emphasize unphysical role of mentioned exchange parameter.

Another question is choice of numerical technique for in surface-subsurface water systems. Cainelli et al. (2012) recently analyzed convergence and approximation properties of common numerical methods for flow and transport analysis in heterogeneous porous media. They defined common methods as the widely used finite element (FEM) and finite volume (FVM) methods. The classic finite element method (FEM) (e.g. Bellin et al., 1992) divides the domain into the finite elements describing the head as a linear combination of classic Lagrangian basis functions (usually linear or quadratic). The inherent problem of the classic FEM methods is discontinuity of head gradients along the inter-element boundaries due to the properties of Lagrangian basis functions. This effect, in combination with the common assumption of the discontinuous conductivity field through the Darcy law, produces numerical “unphysical” velocity discontinuities (variations) causing additional artificial numerical dispersion and for instance inaccurate particle tracking in transport simulations.

Classic FEM can also violate local mass balance over elements. The first way to overcome classic FEM problems is to employ the mixed finite element (MFE) formulation (e.g. Mose et al. 1994), where velocity is also represented by basis functions involving additional degrees of freedom and computational work in flow simulations. Additionally, some MFE formulations can create ill-posed problems. Another way is to perform postprocessor calculations on FEM velocity fields requiring continuity of velocities between elements and/or mass continuation (Yeh et al., 1981; Cordes and Kinzelbach, 1992).

On the other side, FVM methods, such as MODFLOW formulation [e.g. Harbaugh, 2005, de Dreuzy et al., 2007; can also be regarded as cell finite difference formulation], satisfy mass balance over the cell boundaries and ensure velocity continuation normal to the cell boundaries. However, MODFLOW generates discontinuities of tangential velocity components between cells. It is possible to prove equivalence between MODFLOW and MFE which uses low order basis functions (Cainelli et al., 2012).

Gotovac et al. (2009a) presented a such multiresolution approach based on the Adaptive Fup Collocation Method (AFCM) with the following crucial properties: a) correlated log-conductivity ($\ln K$) field is presented as a continuous function in a multiresolution way that can accurately describe all needed scales, b) independently resolves all heterogeneity and head scales, c) yields a continuous velocity field as well as its derivatives needed for application to realistic transport simulations with a velocity dependent dispersion tensor and d) actively controls head and velocity numerical errors reducing numerical dispersion and ensuring convergence, even in highly heterogeneous porous media. The heart of the methodology lies in Fup basis functions (closely related to the B-splines, see Gotovac and Kozulic, 1999) in conjunction with the collocation procedure. However, the main drawback was the lack of local and global mass balance due to the properties of the collocation framework, inability to describe the general irregular geometry and computationally expensive head solution to obtain an accurate velocity field without numerical oscillations for high heterogeneity cases. Among others, applications of the AFCM have been shown for the analysis of the flow and transport in heterogeneous porous media relating to the travel time statistics (Gotovac et al., 2009b), concentration statistics (Srzić et al., 2013) and advective transport (Fiori et al., 2015).

Therefore, in this project, we put desirable AFCM properties to the broader context of isogeometric analysis (IGA). Initially published by Hughes et al. (2005), IGA has attracted enormous attention by designers and modelers because it bridges the gap between Computational Aid Design (CAD) of irregular domains and the numerical description of physical processes on them. The idea is quite simple: use the same type of spline basis functions (usually B-splines or NURBS) to describe both the geometry and solution (head and velocity for our particular groundwater flow problem). IGA has been successfully applied in many fields of solid, structural and fluid mechanics (e.g. Cottrell, Hughes and Bazilevs, 2009). It has been shown that IGA significantly outperforms classical FEM due to higher accuracy and enhanced continuity. Since classic IGA uses the Galerkin variation principle for solution description and transforms the physical domain to the virtual one for geometry description, the apparent similarity between IGA and FEM has resulted in the scientific community widely accepting IGA as new powerful modeling machinery (spline FEM).

In spirit, IGA is closely related to the meshless or mesh-free methodologies due to its use of spline basis functions, which enable many properties not seen in FEM, such as exact geometry description in CAD sense, no classical meshing, more efficient refinement adaptive procedures and multiresolution approach, higher continuity of solution and geometry and usage of higher-order basis functions. Except for the Galerkin weak formulation, IGA recently presented a collocation approach (e.g. Aurichio et al., 2010; Shillinger et al., 2013; Gomez and De Lorenzis, 2016). Recently, our numerical group developed and applied control/finite volume IGA formulation to the groundwater flow modeling in karst aquifers which are representing by 3-D heterogeneous porous matrix and 1-D laminar/turbulent karst conduits (Malenica et al., 2018).

The above-mentioned Multiphysics-fluid problems require large-scale 3-D simulations and highly parallelizable numerical codes. In order to solve realistic 3-D Multiphysics-fluid simulations only viable approach is to use open-source parallel codes/libraries which enable generic and efficient solving of many steps such as: vector-matrix and vector-vector operations, solutions of linear and nonlinear systems, local and global time-stepping, optimization and etc. Some common solutions are PETSc, Trilinos or Hypre (Keyes et al., 2013). Among others, we choose in this project parallel library PETSc (Ballay et al., 2015) and PFLOTRAN (Lichtner et al., 2015) as open numerical code which use PETSc as a main building block. PFLOTRAN lies on robust finite volume parallel code written in Fortran 2003 for surface-subsurface flow and transport processes (the same principles as MODFLOW). In this way, we can create any type of simulations, add our new modules and develop new algorithms on the one side, and use powerful strength of existing codes enabling direct dissemination and recognition of project results to the wider scientific and expert community on the other side.

Lastly, in this project we will devote special attention to the verification of developed new simulations and codes. Using facilities of existing solutions in the literature, our existing laboratory and field measurements as well as new experiments in our new Laboratory for Hydro-Technics in Zrnovnica near Split, all developed numerical solutions will be verified against experimental results. Although different geophysical and other measurement devices tremendously improve ability to measure usually too large data set in real catchments and research areas (see review of Putti and Paniconi, 2015), it is still difficult to measure all critical parts and variables in real surface- subsurface water system. Therefore, we decide to use unique opportunity to verify new algorithms to the exhaustive laboratory data sets.

Section b. The relation of the project proposal to the state of the art in the research area *(describe the relevance of researching the proposed topic, research that you have carried out in this area thus far, the most important results and their relation to the proposed research. Principal Investigators who are already financed by the HRZZ should briefly state the title and objectives of the implemented project, obtained results and its relation to the proposed research.)*

As described in the state of the art in the research field, Multiphysics becomes one of the most important research multidisciplinary area because the most of the unresolved problems cannot be solve using the common separate disciplines and methodologies. Among others, Multiphysics problems in complex water

systems including the interaction of surface and subsurface waters have been already recognized as typical examples where separate analysis do not present realistic and acceptable solutions. Moreover, different problems including additional effects of geomechanics, elasticity, thermodynamics, electricity or radiation can make analysis in multiple water systems even more complex which can be successfully solved only by Multiphysics approach. Very important aspect is bio-cycle of water, mass and energy inside the ecological system confronting interaction of subsurface waters with surface waters from rivers, channels, surface runoff and oceans. Especially, intensive interaction occurs along the coastal regions including mixing of salt and energy inside the complex surface-subsurface water systems.

As described in the Section a) critical points regarding the Multiphysics modelling in surface-subsurface systems are: physical formulations for both parts of the system, coupling between surface and subsurface for flow as well as mass and energy transport, quality and properties of applied numerical techniques, resolving multiscale and multiresolution nature of Multiphysics processes, solving of large problems including more different subdomains and huge number of related equations requiring high parallel computing, related software to be able to solve such heterogenous problems and finally verification and validation of computational models.

Since we keep the standard form of shallow water equations for surface flow and Richards equation for the subsurface flow as well as advection-dispersion equation for mass and energy transport, all other above mentioned consequences in this project will be tried to solve in unique and improved way.

Since the most available surface and subsurface computational models and software lie on control volumes, in the proposed project control volume formulation is chosen due to its conservation properties which is particularly important for accurate transport simulations as tracer tests. Therefore, two options will be used: a) common control volume formulation based on open code PFLOTRAN (Lichtner et al., 2015) and b) novel adaptive Fup multiresolution control volume isogeometric analysis developed by our numerical group (CV-IGA; see Malenica et al., 2018 and Kamber et al., 2018). Since the surface-subsurface systems require different spatial and time scales in order to describe usually fast surface and considerably slower subsurface processes, PFLOTRAN uses unstructured grid for spatial discretization and different time resolutions for both domains, while CV-IGA adaptively finds all resolved spatial and time scales in both domains. In this way, we will have on disposal different approaches to solve the surface-subsurface systems, but keeping the control volume formulation.

Historically, different separate solvers have been developed for surface and subsurface flow and transport processes. Among different possibilities, in this project the generic parallel library PETSc is chosen as basic platform for Multiphysics modeling of the surface-subsurface water systems. PETSc enables solving of the large 3-D nonlinear systems in space and time using parallel computing and object programming. Therefore, the developed methods and new algorithms will be implemented into the parallel open sources codes: (1) 3-D CV-IGA applied with PETSc and (2) PFLOTRAN (new modules) as massively unstructured classic finite volume code for surface-subsurface interactions which also lie on PETSc and Fortran 2003. In this way, project results become visible to the wider community and can be more easily compared with other methods and verified in different large 3-D realistic Multiphysics problems.

Particular project contribution is verification of developed algorithms using controlled laboratory experiments in new Hydrolab in University of Split. Although new measurements and especially new geophysical methods enable enormous progress in measuring large data set for Multiphysics modeling of the surface-subsurface water systems, it is very difficult to control and measure all important segments of the processes under the large catchment scale (order of km²). Therefore, using the very dense set of measuring data in two basins, we will have unique opportunity to verify many properties of SSWS algorithms under strongly controlled laboratory conditions, especially coupling effects and related fluxes between surface and subsurface domains.

For example, surface-subsurface coupled flow problems consist of 3-D porous matrix and usually 1-D surface flow in open channels, rivers or karst conduits, then coupling is often realized by the first-order exchange flux in the form $[q_{ex} = \alpha_{ex}(h_s - h_m)]$ depending on difference between heads in two fluid domains and exchange parameter which is usually constant, obtained from the calibration process and therefore physically meaningful (see our recent results for surface-subsurface flow interactions in karst aquifers, Malenica et al., 2018). Considering exchange flux as separating unknown variable on interface between two flow domains in spite of Lagrangian multiplier (also related to the finite element and volume mortar elements), it is potentially possible to avoid calibration parameters and define interactions in more physical way. Therefore, particular separate discretization is needed in surface and subsurface domain for heads, but also on interface for exchange flux. In this project we will try to define improved coupling strategy based on ideas of Lagrangian multipliers for surface-subsurface interactions, but not only for flow as usual case in the literature. In special designed salt and heat laboratory tracer tests mass and heat transfer coupling needs to be resolved on the laboratory scale between 1-D surface flow and 3-D subsurface flow.

Finally, proposed project results yielding robust parallel 3-D adaptive and verified algorithms will give perspective to the future application to the more realistic catchment scale. Therefore, application of new algorithms in PETSc and PFLOTRAN can be relevant for environmental and ecological modeling analyzing impact of different aspects on eco-system, water-quality, pollution transport, saltwater intrusion in coastal

regions, climate modeling or hydro-power energy. Project results and developed algorithms will be served as platform for further application to different Multiphysics problems, EU projects and other related funds including business sector.

Our previous results are closely related to the research area, especially in the field of isogeometric analysis, subsurface flow and transport numerical and stochastic models and recently karst flow models as examples of surface-subsurface water systems. Our numerical group have developed many numerical algorithms based on spline (especially using Fup basis functions) meshless collocation methods last three decades, for example in structural mechanics (e.g. B. Gotovac and Kozulić, 1999, 2002 or Kozulić and B. Gotovac, 2000, 2017) or fluid mechanics (e.g. Gotovac et al. 2003, 2007). Adaptive multiresolution collocation algorithms for solving the flow and transport subsurface problems was developed in Gotovac et al., 2009a. Further application of mentioned collocation algorithms to the subsurface flow and transport problems in highly heterogeneous porous media are for example presented in the best Water Resources Q1 WoS journals in Gotovac et al., 2009b, 2010, Srzic et al., 2012, 2013a,b, Cvetkovic and Gotovac, 2013, 2014, Fiori et al., 2015).

Recent development was obtained through the Installation Research Project of the Croatian Foundation of Science (in Croatian HRZZ) – UIP-2013-8103 which called “Groundwater flow modeling in karst aquifers” from 01/10/2014 to 01/02/2019. In that project control volume isogeometric formulation (CV-IGA) is developed for the first time (Kamber et al., 2018).

Also, the karst flow model is developed and verified on 3-D sandbox which is now located in the front of new Hydrolab in Zrnovnica (Malenica et al., 2018). A discrete-continuum (hybrid) approach, in which a three-dimensional matrix flow is coupled with a one-dimensional conduit flow, was used. The laminar flow in the karst matrix is described by a variably saturated flow equation to account for important hydrodynamic effects in both the saturated and unsaturated zones. Turbulent conduit flow for both free surface and pressurized flow conditions was captured via the noninertia wave equation, whereas the coupling of two flow domains was established through an exchange term proportional to head differences. The novel numerical approach based on Fup basis functions and control-volume formulation enabled us to obtain smooth and locally conservative numerical solutions. Due to its similarity to the isogeometric analysis concept (IGA), we labeled it as control-volume isogeometric analysis (CV-IGA). Since realistic verification of the karst flow models is an extremely difficult task, the particular contribution of this work is the construction of a specially designed 3D physical model (dimensions: $5.66 \times 2.95 \times 2.00$ m) in order to verify the developed numerical model under controlled laboratory conditions. Heterogeneous porous material was used to simulate the karst matrix, and perforated pipes were used as karst conduits. The model was able to capture many flow characteristics, such as the interaction between the matrix and conduit, rainfall infiltration through the unsaturated zone, direct recharge through sinkholes, and both free surface and pressurized flow in conduits. Two different flow experiments are presented, and comparison with numerical results confirmed the validity of the developed karst flow model under complex laboratory conditions.

All main project results are presented in PhD Thesis of Malenica (2019). Additional project result was development of an adaptive multiresolution method based on new hierarchical Fup basis functions and CV-IGA (initial 1-D results are presented in Kamber et al., 2018). Among other interesting properties, the novel adaptive CV-IGA introduced k-refinement as advanced version of local hp-refinement, because any basis function of the n-th order from one resolution level can be replaced by a linear combination of more basis functions of the n+1-th order at the next resolution level providing spectral convergence order. 2-D steady-state adaptive results will be published in new articles and PhD Thesis of Grgo Kamber which is planned to be defended until the end of this year. In the one-year post-project phase, three papers are currently in the last stage of the peer review process.

All these results prove that our group is able to produce another step toward to more advanced Multiphysics modelling of surface-subsurface water systems using the unique numerical properties of new hierarchical Fup basis functions and CV-IGA, powerful parallel capabilities of open source codes PETSc and PFLOTRAN as well as controlled laboratory experiments in new Hydrolab in Zrnovnica with respect to the institutional support of FGAG and ORNL.

Section c. Methodology *(please describe the research methodology in detail. Please state and describe in detail the planned analyses and procedures, the equipment to be used, number and type of samples, examinees, their characteristics or area of research.)*

Multiphysics SSWS problems require 3-D parallel large-scale PDE-based numerical simulations. As already explained, novel algorithms for SSWS based on classic control volume or more advanced CV-IGA will be incorporated to the open source libraries PETSc and PFLOTRAN which enable such powerful numerical simulations.

New SSWS algorithms will lie on the control volume methodology which enables local and global mass and/or flux conservation and fewer efforts for numerical integration in comparison to FEM. SSWS algorithms will use discrete-continuum (hybrid) approach, in which a three-dimensional subsurface matrix flow and

transport is coupled with a one and two dimensional surface flow and transport. 1-D surface flow describes flow in channels, rivers or karst deep conduits. 2-D surface flow describes runoff flow over the upper surface of the domain or fracture flow in fractured (karstified) porous medium. Mathematical model for subsurface flow is described by Richards nonlinear equation which presents unsaturated flow conditions. Mathematical model for surface flow is described by shallow water equations or usually by its simpler version using the nonlinear diffusive wave equation (Malenica, 2019) which can describe laminar and turbulent flow as well as pressurized or free flow. Mass and energy transport in both domains are described by well known advection-dispersion equation.

We will use classic control volume formulation in PFLOTTRAN (Lichtner et al., 2015) which uses one unknown variable per control volume/cell, while fluxes are calculated by low order finite-difference expressions. Time stepping procedure is usually obtained by implicit Euler unconditionally stable scheme. It is basically very stable second order algorithm. PFLOTTRAN is initially written for subsurface flow and reactive parallel simulations. There are also surface, geo-mechanics and few more modules in order to run different Multiphysics simulations. Generally, other modules are not so sophisticated as main subsurface module. In objectives O2 and O3 we will need to improve these modules and construct improved coupling strategy and connect surface and subsurface modules via fluxes on the interface between two flow domains. These new modules in PFLOTTRAN will be modelling project contribution. It will be verified by flow and tracer tests originally produced in our new Hydrolab. In objective O4 geomechanics module will be connected to the subsurface module in order to simulate hydro-mechanical Multiphysics problems. It will be verified by known examples from the literature. In this way, application of PFLOTTRAN will cover all simulation in O2-O4.

PFLOTTRAN is based on parallel library PETSc (Portable Extensive Toolkit for Scientific Computations; Balay et al., 2015) which is a main building block for parallelism where developer-scientist do not need to worry about MPI and production of stand-alone parallel coding. Rather, developer can put focus on physics and other method details. PETSc solves large sparse linear systems by Krylov subspace methods such as conjugate gradients, GMRES and BiCGstab. Efforts are needed to find appropriate preconditioner which can significantly speedup simulations. For example, for PFLOTTRAN and subsurface simulations, additive Schwartz preconditioner (based on block-Jacobi) can be very robust option (see Gotovac et al., 2009a). Moreover, PETSc also can solve nonlinear systems via different type of Newton methods and time integration via different time-stepping implicit schemes. In this project we will use CPU and GPU versions of PETSc. Graphical preprocessing for preparation of discretization, geometry, materials, initial and boundary conditions and generally input data and postprocessing for visualizing velocities, fluxes, heads and concentrations will be performed on new GPU node using well known postprocessor Tecplot and powerful pre and post processor GiD.

Also, our mentioned novel CV-IGA formulation will be incorporated in PETSc. Solution as well as geometry and material are obtained by linear combination of spline/Fup basis functions. Now, solution and its derivatives (fluxes) are presented as functions, not as discrete values in classic form of PFLOTTRAN. In this case, there is one basis function coefficient as unknown variable per each control volume. Algorithm is now higher-order and can use hierarchical Fup basis functions with above mentioned efficient adaptive procedures. Also, coupling strategy inside CV-IGA will be key element for its application to the SSWS problems and therefore significant project contribution.

All numerical algorithms will be verified by extensive experimental laboratory measurements. For experimental SSWS results, we have flow (Malenica et al., 2018) and tracer (currently underway) experiments in existing sandbox (4*2.5*2m) in Zrnovnica (also funded by HRZZ). However, we will have new larger sandbox (22*4*2.6m) in new Laboratory in Zrnovnica near Split (planned opening is 1.1.2021.) with extensive equipment including 360 pressure and 120 concentration and temperature sensors in order to perform unique tracer tests. In this project we will perform salt and heat tracer tests to verify simulations of surface-subsurface interactions. Simultaneously, we will measure flow variables such as flow rates in porous matrix and channels/conduits or heads in piezometers as well as transfer of salt and heat using 120 sensors for measuring electrical conductivity and temperatures. Additionally, rainfall station above both 3-D sandboxes can produce desired level of precipitation and can be useful for investigation of runoff or enhanced flow and transport in karst conduits. All measurements will be obtained in real time and stored in the cluster. Number of experiments will be coordinated with quality of numerical verification and unsolved effects.

In project we will also perform additional measurements by ERT (electrical resistivity tomography). Particularly, electric resistivity tomography (ERT) is special type of geophysics methods for locating of spatial distribution of salt tracers in different time intervals. Since pressure, concentration and temperature sensors enable point data in space, but continuous record in time, ERT enables opposite, spatial distribution of tracer distribution in discrete time intervals. ERT can define heterogeneity with respect to the hydraulic conductivity of sandbox and tracer conditions prior to the tracer test. Measuring in different time intervals can infer salt spatial distribution due to difference between records among different time intervals.

In this project we will use conservative salt and heat tracer tests. In that case tracers are simple mixture of salt and fresh water or heating water. Since we have extensive experimental equipment for pressure and concentration – electrical conductivity, it is possible to conduct flow and salt tracer tests. However, additional proposed temperature measurements enable heat tracer tests which are complementary to the salt tracers and yield additional information about surface-subsurface interactions. Also, tracer is only heating water, relatively inexpensive experiment which enables much more data than only salt tracing. Except advection and dispersion, conduction between heat tracer water and solid phase is also important additional process which is not present for salt tracers. It means that proposed tracer tests are mutually complementary.

Finally, in this project extensive and sophisticated experimental and numerical methods will be used. Their integration will provide better understanding of project results and future application of developed algorithms.

Section d. Research impact *(describe the expected impact of the research. Describe the expected impacts of the research and contribution to the area of research and/or development of society and the economy. In case of applied research, describe the potential needs for utilising research results, the groups of potential beneficiaries and the effects that can be expected in the case of their application).*

Multiphysics creates new avenues for emerging scientific disciplines and solution approaches to physical and engineering problems. Multiphysics does not mean separate treatment of physical components, rather it is a new integrated physical system with new properties. Particularly, Multiphysics-water complex systems present a very important field not only for the above-mentioned environmental issues, but also a platform for development of new industrial technologies and products. Small countries such as Croatia usually cannot ensure facilities for massive industry but developed algorithms and tools such as PFLOTTRAN can be employed for development of new special technologies needed for creation of small and medium enterprises.

Our project results may be very important for Croatian water resources. For example, catchment of river Jadro supplies Split large urban agglomeration of 300 000 habitants. New algorithm in PFLOTTRAN developed in this project can be used for analysis of flow and transport in that karst aquifer. Temporarily, there is no such application for this important water body. Another example is Neretva valley, an important agricultural region with a problem of saltwater intrusion in upper sand-gravel sub-aquifer.

Project results open lot of space for application to many other Multiphysics (not only fluid) inter-disciplinary problems. Furthermore, scientific cooperation between FGAG and ORNL, further cooperation with other EU partners as well as resources of FGAG (new laboratory in Zrnovnica) and ORNL (1-st supercomputer in the world) are solid basis for further application to EU funds, but also to other projects between USA and EU. Particular opportunities are EU funds such as Interreg IPA projects which enable scientific, but also high-level engineering development. Also, there are lot of EU funds for joint projects with business sector. Currently, we have applications to IRI project with CEMEX company for permeable concrete surface areas. Project results are tools for future research and application in similar applied projects.

Potential stakeholders of proposed research are public companies such as Croatian Waters, public authorities, Croatian Electrical and Water Supply companies, environmental agencies, but also many small and medium enterprises who are potentially interested for innovations and technologies related to the Multiphysics-water modelling.

Section e. Work Plan *(This section of the Project Proposal should clearly show how the planned project objectives will be accomplished. Please describe the research approach; the proposed research objectives, results and their connection to the resources by abiding to the proposed structure.)*

d1. Objectives *(specify and describe the scientific objectives of the proposed research.)*

The overarching objective of this project is to develop new scalable parallel coupling algorithms for Multiphysics fluid systems. In order to achieve this goal, the following project objectives are proposed:

Objective – O1: Adaptive modelling based on hierarchical Fup basis functions and isogeometric analysis

During the last 15 years, IsoGeometric Analysis (IGA) has attracted enormous attention in numerical modeling due to properties of spline basis functions to describe both, irregular geometry in CAD meaning and problem solution (Hughes et al., 2005). Classical IGA uses B-splines and NURBS inside weak Galerkin formulation which presents so-called spline-FEM. Cortrell et al. (2009) presented that IGA generally enables higher-order solutions, continuous fluxes and significantly better approximation properties than classical FEM based on Lagrangian basis functions. Except weak Galerkin and strong collocation formulation, we recently developed weak CV-IGA (control volume) formulation (Malenica, 2019). Among others, particular property of IGA is efficient construction of adaptive multiresolution algorithms based on hierarchical B-splines in

comparison with classic FVM and FEM. Our research group at University of Split has been developing adaptive algorithms based on Fup basis functions which are infinitely derivable or perfect splines (e.g. Gotovac et al., 2009). Our present PhD student Grgo Kamber (also funded by HRZZ) introduced new hierarchical Fup basis functions within CV-IGA and applied them to the 1-D problems (Kamber et al., 2018). These first results show that hierarchical Fup's outperform hierarchical B-splines because they enable exponential convergence (B-splines enables only classic polynomial convergence) and h-p adaptive procedure (contrary to h-adaptation by B-splines) which means that higher resolution levels not only add basis functions with smaller compact support or higher frequencies, but also increase order of basis functions. In this way, solution is described with optimal number of basis functions using different resolution levels inside domain on adaptive control volume grid. Therefore, this novel adaptive procedure has significant potential for the application of mentioned Multiphysics-fluid problems. This objective leads to the construction of 2-D and 3-D adaptive algorithm with novel hierarchical Fup basis functions within CV-IGA. Finally, methodology needs to be accommodated for surface-subsurface tracer tests. Moreover, this new algorithm will be implemented in the open source code PETSc.

Key activities in the 1-st project period: write and develop 2-D unsteady adaptive CV-IGA algorithm in Fortran using the PETSc, define space and time discretization, define preconditioners and nonlinear solver, verify algorithm to the known examples in the literature and prove convergence in space and time, write and present scientific conference paper.

Key activities in the 2-nd project period: write and develop 3-D unsteady adaptive CV-IGA algorithm in Fortran using the PETSc, define time space and discretization, verify algorithm to the known examples in the literature and prove convergence in space and time, write and publish scientific WoS journal paper.

Key activities in the 3-rd project period: define coupling implementation of fluxes between surface and subsurface domains using adaptive CV-IGA, define iterative procedure to solving Multiphysics in both domains, implement algorithm to PETSc, verify algorithm to the tracer tests from objectives O2 and O3, write and publish scientific WoS journal paper and one conference paper.

Objective – O2: Multiphysics modeling of tracer tests in river-channel-subsurface systems

This objective will develop a new algorithm for integrated surface-subsurface hydrological systems consisting of 1-D channels/ivers, 2-D overland surface flow as well as 3-D porous matrix. The algorithm will be incorporated in open source code PFLOTRAN (classic finite volume approach) which will make it available to the expert and scientific communities. PFLOTRAN implementation will enable solving of large-scale problems with help of PETSc and stable algorithms due to application of low-order classical methods. The new algorithm will have improved coupling strategy, adaptive (unstructured) spatial grid in each domain and different time-stepping in fast surface and slow subsurface flow domains. A particular significance will be given to verification against the flow experiments in the new 3-D experimental setups for river-channel-runoff-matrix coupling. Moreover, in this objective we will develop new tracer tests based on salt and heat tracers which will be performed in the new Laboratory at University of Split. Verification under controlled laboratory conditions will promote reliability of these Multiphysics complex simulations. In this way, a new algorithm will present significant modeling improvement for SSWS, especially for further application to the real systems.

Key activities in the 1-st project period: create modules in PFLOTRAN for flow coupling between surface and subsurface flow, perform new flow tests in new large 3-D sandbox, verify new modules on flow tests, write and present scientific conference paper.

Key activities in the 2-nd project period: perform new heat and salt tracer tests in new large 3-D sandbox, verify new modules on tracer tests, write and present scientific conference paper.

Key activities in the 3-rd project period: perform new heat and salt tracer tests in new large 3-D sandbox, verify new modules on tracer tests, write and present scientific conference paper, write and publish scientific WoS journal paper.

Objective – O3: Multiphysics modeling of tracer tests in karst systems

This objective will develop a new algorithm for integrated surface-subsurface karst systems consisting of 1-D conduits as well as 3-D porous matrix. The algorithm will be incorporated in open source code PFLOTRAN (classic finite volume approach) which will make it available to the expert and scientific communities. PFLOTRAN implementation will enable solving of large-scale problems with help of PETSc and stable

algorithms due to application of low-order classical methods. The new algorithm will have improved coupling strategy, adaptive (unstructured) spatial grid in each domain and different time-stepping in fast surface and slow subsurface flow domains. A particular significance will be given to verification against the flow experiments in the old 3-D experimental setups for conduit-matrix coupling. Moreover, in this objective we will develop new tracer tests based on salt and heat tracers which will be performed in the old 3-D sandbox. Verification under controlled laboratory conditions will promote reliability of these Multiphysics complex simulations. In this way, a new algorithm will present significant modeling improvement for SSWS, especially for further application to the real karst systems such as Jadro.

Key activities in the 1-st project period: create modules in PFLOTTRAN for mass and heat transport coupling between surface and subsurface flow, perform new tracer tests in old 3-D sandbox, verify new modules on flow and tracer performed tests.

Key activities in the 2-nd project period: perform new heat and salt tracer tests in old 3-D sandbox, verify new modules on tracer tests, write and publish scientific WoS journal paper.

Key activities in the 3-rd project period: perform new heat and salt tracer tests in old 3-D sandbox, verify new modules on tracer tests, write and present scientific conference paper.

Objective – O4: Multiphysics modeling of hydro-mechanical systems

This Objective is complementary objective with first three objectives. In this case, an improved coupling strategy will be applied to the interface between the pore and solid phase inside the same domain - porous medium. It means that coupling should be performed between geomechanics and subsurface module in PFLOTTRAN.

Key activities in the 1-st project period: create modules in PFLOTTRAN for coupling between geomechanics and subsurface module, verify new modules on the examples for the literature.

Key activities in the 2-nd project period: verify new modules on the examples for the literature, write and publish scientific WoS journal paper.

Key activities in the 3-rd project period: verify new modules on the examples for the literature, write and present scientific conference paper.

Objective – O5: Dissemination

Dissemination is an important task in this project which will be completely presented in project web pages. All previously mentioned objectives create results which will be implemented into open source codes PFLOTTRAN and PETSc. In this way, the project results are ready for further applications; all verification tests (related to experimental data) are freely approachable for all users since it is the fastest and the most visible way for wider expert and scientific community. Moreover, all results will be presented in journal papers and scientific conferences. Also, we will prepare special Tribune – “Multiphysics-fluid” for Science Festival of University of Split to present project results to the wider population such as pupils, ordinary people, ecology groups, etc, in spirit of popularization of science. Finally, at the end of the project, Final Workshop will be organized in order to present all project results to the expert and scientific community as well as other stakeholders such as ecological organizations or public companies as Government departments, HEP, Croatian Waters, VIK, IGH and some others.

d2. Expected results (specify planned results for each research objective.)

Objective O1

1 conference presentation and 1 journal paper in Q1/Q2 WoS journals related to the 2-D and 3-D unsteady algorithm based on application of hierarchical Fup basis functions and adaptive CV-IGA in PETSc.

1 conference presentation and 1 journal paper in Q1/Q2 WoS journals related to the 3-D application of hierarchical Fup basis functions and adaptive CV-IGA in PETSc to flow and tracer tests developed in O2 and O3.

Open source code in PETSc.

Potential users are expert and scientific community.

Objective O2

1 conference presentation related to the construction of the modules for flow in surface-subsurface hydrological systems inside open source-code PFLOTRAN and application of the new algorithm to the existing flow laboratory data.

2 conference presentation and 1 journal paper in Q1/Q2 WoS journals related to the construction of the modules for flow and transport in surface-subsurface hydrological systems inside open source-code PFLOTRAN and application of the new algorithm to the tracer laboratory data .

Open source code in PFLOTRAN with new modules for Multiphysics modeling of flow and transport problems in surface-subsurface systems.

Potential users are expert and scientific community.

Objective O3

2 conference presentation and 1 journal paper in Q1/Q2 WoS journals related to the development of new algorithm for flow and transport in surface-subsurface karst systems verified on flow and tracer test in old 3-D sandbox.

Open source code in PFLOTRAN with new modules for Multiphysics modeling of flow and transport problems in surface-subsurface karst systems.

Potential users are expert and scientific community.

Objective O4

1 conference presentation and 1 journal paper in Q1/Q2 WoS journals related to the development of new algorithm for interaction between geomechanics and subsurface module in PFLOTRAN.

Open source code in PFLOTRAN with new modules for Multiphysics modeling of hydro-mechanical systems.

Potential users are expert and scientific community.

Objective O5

2 PhD dissertations of two PhD students (Potential users are expert and scientific community).

Tribune "Engineering numerical modeling of Multiphysics-fluid complex systems" presented on Science Festival at University of Split in spirit of popularization of science (Potential users are pupils, ordinary people and wider population).

Final project Workshop for presentation of all project results (oral presentation, posters, flyers). Potential users are expert and scientific community as well as stakeholders such as ecological organizations or public companies as Government departments, HEP, Croatian Waters, VIK, IGH and some others.

Project web pages for direct presentation and visualization of developed algorithms for wider experts and engineers who will use developed algorithms.

Application of new algorithm in PFLOTRAN and PETSc can be relevant for environmental and ecological modeling analyzing impact of different aspects on eco-system, water-quality, pollution transport, saltwater intrusion in coastal regions, climate modeling or hydro-power energy. Multiphysics-fluid developed algorithms can be applied in many existing and new industrial problems and specially for development of new technologies.

d3. Describe *potential risks* of the proposed research and the action plan should the mentioned risks occur.

Potential risk for the proposed project can be problems in the implementation of EU infrastructure project „INFRA“ for construction of new Hydrolab at FGAG. However, we have existing smaller sandbox in Zrnovnica in order to compensate planned new experiments. Also, there could be always possible problems with work, motivation and progress of current and new PhD and Postdoc students. We will try to make positive work atmosphere and fix problems as soon as it becomes more serious. Finally, risks exist in the process of the equipment purchasing in case of possible complaints and repetition of procedures which can create time delay of some experimental activities. We will try to solve that issue by carefully prepared tender documentation leaving small space for possible misunderstanding and undefined details.

Section f. Resources (describe the costs of the proposed project in HRK, including the material resources that shall be provided by the Institution for the purpose of implementing the research. Please state all additional sources of funding

and all project proposals submitted or peer reviewed which are in connection with the implementation of the proposed research. Specify the proposed project budget by linking the items in the financial plan with the corresponding objectives, deliverables and activities. Explain all the items in the financial plan. The budget needs to be accurate and clearly specified. Please state the percentage of the working hours which the applicant will dedicate to the project implementation.

Note: In order to simplify the evaluation panel's task of assessing the resources, the information listed in the Financial Plan should also be replicated in the description of the resources.)

Financial plan is heavily based on the resources of our institution – FGAG. FGAG will support this project with new laboratory for Hydro-technics in Zrnovnica near Split. Total value of equipment is 16.500.000,00 HRK inside new building worthy of 15.000.000,00 HRK. There are four main parts of the new HydroLab: 1) Water flume (26 m) with cross section of 1.2*0.6 m, wave generator and PIV/LIF system for measurements 3-D velocity and 2-D tracer concentration, 2) Wind tunnel of closed type with work section (0.6*0.65 m) and PIV/LIF, 3) 3-D sandbox (10*4*2 m) with precipitation station, 480 piezometers, 360 pressure and 120 concentration sensors, 4) Basin (11*4*2 m) with wave generator. In this project we will use 3-D sandbox for surface-subsurface flow and transport modeling for objectives O1 and specially O2.

FGAG has computer cluster with 6 CPU nodes and 144 cores. It is small cluster, particularly suited for development of algorithms and related codes, as in the proposed project for all objectives O1-O5. For realistic 3-D large-scale parallel Multiphysics simulations, larger resources are needed.

ORNL-Oak Ridge National Laboratory is our collaboration institution and has the largest computer resources in the world. At latest list of ten the largest world supercomputers (<https://www.networkworld.com/article/3236875/servers/embargo-10-of-the-worlds-fastest-supercomputers.html>), ORNL has two supercomputers: Summit (over than 2 000 000 CPU/GPU cores) at the first place and Cray xk7- Titan with NVIDIA k20x GPU accelerators at 9-th place. In this project we will have opportunity to utilize such exhaustive resources depending of project results and our needs.

Finally, FGAG has one more important resource for proposed project. Firstly, there is smaller 3-D sandbox (4*2.5*2 m) with 50 pressure sensors and 4 concentration sensors (objective O3). Flow simulations are recently published (Malenica et al., 2018) while new tracer tests will be obtained in objective O3.

Total proposed project budget is almost 1.500.000,00 HRK.

Except older researchers, there are two existing PhD students and two new Postdoc who will be paid by project budget (2+2 years). Almost half budget in Category 2 will be spent for their salary and other related costs including the PhD student tuition fee for Assistant Krste Živković. PhD students will devote 60% of the work time, while two new Postdoc will spend 90% work time to the project activities. All other older researchers will devote 25% of their work time to the project.

In category 1. Research costs, small material supply (17.000,00 HRK) is needed to perform flow and tracer tests in new HydroLab. Also, additional services are needed for installation of new cluster equipment nad their maintenance (42.000,00 HRK). Supporting consulting and expertise are needed for covering special project activities such as IT expertise for maintenance of cluster and installation of GPU nodes which require special knowledge for Linux operating systems as well as for creation and web pages which will increase project visibility (8.000,00 HRK). Particularly, electric resistivity tomography (ERT) is special type of geophysics methods for locating of spatial distribution of salt tracers in different time intervals. Since pressure, concentration and temperature sensors enable point data in space, but continuous record in time, ERT enables opposite, spatial distribution of tracer distribution in discrete time intervals. ERT can define heterogeneity with respect to the hydraulic conductivity of sandbox and tracer conditions prior to the tracer test. Measuring in different time intervals can infer salt spatial distribution due to difference between records among different time intervals. Such measurements can be done only by special licensed companies equipped with ERT geophysics instruments. Nine measuring campaigns will cost 200.000,00 HRK. These ERT measurements are needed for objectives O1-O3. This category is covered by field research in Jadro catchment (20.000,00 HRK) and purchasing of scientific literature (6.000,00 HRK).

In category 3. Equipment costs, another important new equipment upgrading is two GPU nodes which will be installed in the existing cluster at FGAG. Since cluster has only 6 CPU nodes, this new upgrading will enable usage of PETSc both, on CPU and GPU nodes which is compatible with mentioned ORNL supercomputers. One new GPU node will consist of 12 CPU cores and one GPU card NVIDIA Tesla T4 16GB with 2560 GPU cores. Moreover, second GPU node and upgrading of software – Tecplot and GID for only graphical pre and postprocessing will be installed. This upgrading is important for all objectives O1-O5.

In category 4. Training dissemination and publications costs, proposed project will cover travel, fees, accomodation and other costs for different activities: a) two week training at ORNL - partner organization which will ensure coordination of all project activities and especially work for implementation new modules in PFLOTRAN and PETSc (70.000,00 HRK), b) attendance to seven international scientific conferences will ensure dissemination of results, c) organization of final project Workshop will present all results for wider

community and different interested stakeholders (8.000,00 HRK), d) organizing of the 1-st International Conference on atomic and R-functions by Principal Investigator will promote preject activities and especially CV-IGA and new hierarchical Fup basis functions and e) publication costs for acces open journals in order to better and faster present project results to scientific community 40.000,00 HRK). This Category spent maximum money, 70.000 HRK per year.

Section g. Ethical issues

There are no problematic ethical issues in the proposed project.

Section C – Research Group

List all persons who will be involved in the implementation of the proposed research (please specify the associates (S), PhD students (D)*, postdoctoral researchers (P)* who will be employed on the project)						
Name and surname	Title	Institution	Country	Year of PhD award (if applicable)	Role within the project (S, D, P)	Percentage of working hours spent on the proposed project
Vedrana Kozulić	PhD, Professor	Faculty of civil engineering, Architecture and Geodesy (FGAG)	Croatia	1999	S	25%
Blaž Gotovac	PhD, Professor	(FGAG)	Croatia	1987	S	25%
Ivan Đepina	PhD, PostDoc	(FGAG)	Croatia	2016	P	25%
Grgo Kamber	PhD student	(FGAG)	Croatia		D	60%
Krste Živković	PhD student	(FGAG)	Croatia		D	60%
Postodoc I	PhD	(FGAG)	Croatia		P	90%
Postodoc II	PhD	(FGAG)	Croatia		P	90%

* for the doctoral students and/or postdoctoral researchers who are not employed at the time of application but their employment is planned by the project, please put in the „name and surname“ column their role in the project and add the percentage of the planned working time on the project.

Section a. Research group (specify their roles and tasks in the project implementation)

Vedrana Kozulić	S, Researcher for objective O1
Blaž Gotovac	S, Researcher for objective O1
Ivan Đepina	P, Researcher for objective O4
Grgo Kamber	D, Researcher for objective O1, O2
Krste Živković	D, Researcher for objectives O1-O3
Postodoc I	P, Researcher for objectives O1-O2
Postodoc II	P, Researcher for objectives O1-O3

Section b. Curriculum Vitae of team members, i.e. role profiles and competencies of the team members who will be employed during the implementation of the project (The format of the Curriculum Vitae should adhere to the structure of the *Track Record*, Section A of this document. Please add rows as needed).

Name and surname: Vedrana Kozulić, Scientist identification number²: 176112

Curriculum Vitae (max. 1 page)

Date of birth: 13. January 1962. Nationality: Croatian. Name of employer: University of Split, Faculty of Civil Engineering, Architecture and Geodesy, Department of Technical Mechanics. Type of business: Professor (since 2010.). Position held: Chief of Department of Technical Mechanics. Title Master of technical science: 1993. (title of thesis: Numerical analysis of structures consisting of shells and columns). Title Ph. D. of technical science: 1999. (title of thesis: Numerical modelling by the fragment method with Rbf functions). Research subjects: structural mechanics, engineering structures, numerical modelling of linear and nonlinear problems. Member of professional associations: Croatian Society of Mechanics, Central European Association for Computational Mechanics (CEACM), Society of civil engineers Split, European Mechanics Society (EUROMECH). Speaking and writing: English language. The list of research projects funded by MSES in the Republic of Croatia in which the team member Vedrana Kozulić was involved are: Nonlinear numerical modelling of civil engineering structures (2-11-054) (1991.-1996.), Numerical modelling of engineering structures (083133) (1997.-2000.), Numerical modelling of spatial engineering structures (083132) (2000.-2002.), Modern numerical modelling of tunnels and underground structures (0083041) (2002.-2005.), Numerical modelling of quasi-brittle materials (0114002) (2002.-2005.). Research project funded by Croatian Science Foundation in which the team member Vedrana Kozulić was involved: Groundwater flow modeling in karst aquifers (HRZZ-UIP-2013-11-8103) (2014.-2017.).

Vedrana Kozulić was principal investigator in the scientific project funded by MSES in the Republic of Croatia. Name of this project is "Adaptive meshless modeling in design of engineering structures" (083-0831541-1534) (2007.-2013.). The main purpose of the project was representation of the role of atomic basis functions in the field of numerical mechanics. She published 65 scientific papers, among them 5 papers published as chapters in scientific books with an internationally recognized review indexed into databases Cambridge Scientific Abstracts, INSPEC, Google Scholar and Scopus, 8 papers in CC journals and SCI, SCIEExpanded bases, 3 scientific papers in journals with an internationally recognized review indexed in other bases, 6 papers in the other journals, 30 papers in Proceedings of International meetings. She had three invited lectures at international conferences, 15 lectures at international conferences and 6 lectures at national conferences. Her published scientific papers were cited 68 times according to the largest abstract and citation database of peer-reviewed literature SCOPUS.

Complete list of published scientific papers on the link:

<https://www.scopus.com/results/results.uri?sort=plff&src=s&st1=Kozulic&st2=V.&nlo=1&nlr=20&nls=afprfnmt&sid=edbed0cff3787e192332454322ca297c&sot=anl&sdt=aut&sl=36&s=AUID%28%22Kozuli%2c%22+Vedrana%22+7801669505%29&partialQuery=&txGid=6e0e9e5dee75bf7e650f392285d6df30>

²Registration number generated upon registering in the Register of Researchers of the Ministry of Science and Education.

Name and surname: Blaž Gotovac, **Scientist identification number:** 014020

Curriculum Vitae (max. 1 page)

Date of birth: 22. January 1951. Nationality: Croatian. Name of employer: University of Split, Faculty of Civil Engineering, Architecture and Geodesy, Department of Technical Mechanics. Type of business: Professor (since 2002.). Title Master of science in civil engineering: 1982. (title of thesis: Analysis of the plane problem in elastic and hydrodynamic porous media). Title Ph. D. of technical science: 1987. (title of thesis: Numerical modelling of engineering problems by smooth finite functions). Research subjects: structural mechanics, engineering structures, numerical modelling of linear and nonlinear problems, development of procedures for the reconstruction of cultural heritage objects. Member of professional associations: Croatian Society of Mechanics, Society of civil engineers Split, Croatian Society of Geotechnics. The list of funded research projects in which the team member Blaž Gotovac was involved are: Stability of spatial engineering structures (1983.-1984.), Numerical model of material behaviour with propagation and monitoring of fractures (1983.), International educative project TEMPUSICADERS (Integrated CAD of Earthquake Resistant Buildings and Civil Engineering Structures) (1992.-1995.), Adaptive meshless modeling in design of engineering structures (083-0831541-1534) (2007.-2013.), Groundwater flow modeling in karst aquifers (HRZZ-UIP-2013-11-8103) (2014.-2017.). Blaž Gotovac was principal investigator in the following scientific projects funded by MSES in the Republic of Croatia: Numerical modelling of surface structures (2-11-293) (1991.-1996.), Numerical modelling of spatial engineering structures (083132) (2000.-2002.), Modern numerical modelling of tunnels and underground structures (0083041) (2002.-2005.). He published 72 scientific papers, among them 5 papers published as chapters in scientific books with an internationally recognized review indexed into databases Cambridge Scientific Abstracts, INSPEC, Google Scholar and Scopus, 10 papers in CC journals and SCI, SCIEExpanded bases, 3 scientific papers in journals with an internationally recognized review indexed in other bases, 9 papers in the other journals, 30 papers in Proceedings of International meetings. He had 5 invited lectures at international conferences, 10 lectures at international conferences and 12 lectures at national conferences. His published scientific papers were cited 100 times according to the largest abstract and citation database of peerreviewed literature SCOPUS. He reviewed scientific papers in many journals.

Complete list of published scientific papers on the link:

<https://www.scopus.com/results/results.uri?sort=plff&src=s&st1=Gotovac&st2=B.&nlo=1&nlr=20&nls=afprfnmt&sid=5aa3331e46d9716f83aa96fda64a192b&sot=anl&sdt=aut&sl=33&s=AUID%28%22Gotovac%2c+Bla%2c%5be%22+6602441620%29&partialQuery=&txGid=e7398db9a0565e5e29dfa3cc358cceb>

Name and surname: Ivan Đepina, **Scientist identification number:** --

Curriculum Vitae (max. 1 page)

Education

2012–2016 PhD Degree, Norwegian University of Science and Technology, Department of Civil and Transport Engineering, Trondheim, Norway, Topic: Reliability Analysis of Monopile Foundations for Offshore Wind Turbines.

2009–2011 Master Degree in Civil Engineering,

University of Split, Faculty of Civil Engineering, Architecture and Geodesy, Split, Croatia.

2006–2009 Bachelor Degree in Civil Engineering, University of Split, Faculty of Civil Engineering, Architecture and Geodesy, Split, Croatia. Academic and research experience

2012–2016 PhD Candidate, Norwegian University of Science and Technology, Department of Civil and Transport

Engineering, Trondheim, Norway.

2014–2016 Associate Profesor/University lecturer, Norwegian

University of Science and Technology, Department of Civil and Transport Engineering,

Trondheim, Norway. Course Geohazards and Risk Analysis 2016–present Researcher, SINTEF Infrastructure, Trondheim, Norway.

2018–present Postdoctoral fellow, University of Split, Faculty

of Civil Engineering, Architecture and Geodesy, Split, Croatia, Research topic: Fluid-structure interaction.

Dissertations

Depina, Ivan. (2016) Reliability analysis of monopile foundations for offshore wind turbines. PhD thesis at NTNU (2016:171), ISBN 978-82-471-4196-0.

Depina, Ivan. (2011) Seismic resistance of masonry buildings. Master thesis at University of Split, Faculty of Civil Engineering, Architecture and Geodesy (624.042).

Journal publications

Published 7 WoS journal papers.

Awards and honors

Award for excellence on the national level in Croatia, 2011 + Rector Award. Award for excellence at the University of Split, Croatia, 2009/10 + Dean Award. Award for excellence at the Faculty of Civil Engineering Architecture and Geodesy, Split, Croatia, for years 2007/08, 2008/09, and 2009/10

Conference publications

Published 13 scientific papers in international scientific conferences.

Projects

He participated in 7 international scientific projects.

Name and surname: Krste Živković, **Scientist identification number:** ----

Curriculum Vitae (max. 1 page)

Born: 14.06.1979.

Residence: Šibenik / Šibenik

Married and father of two kids

Education

1997-2005 – FGAG (Bachelor Degree-low level)

2008 – 2010 – FGAG (Bachelor Degree)

Work experience

2005. - 2006. "Zmajevo oko-Rogoznica" d.o.o.

2008. "Krak" d.o.o.

2011. - "Komunalno poduzeće" d.o.o. Knin

2019 – present – PhD student at FGAG

Name and surname: Grgo Kamber, Scientist identification number: 361714

Curriculum Vitae (max. 1 page)

Date of birth: 27. August 1990 in Split. Nationality: Croatian. Finished primary and high school in Split. After graduating from high school, enrolled in the university undergraduate study of civil engineering academic year 2009./2010. 2012./2013. enrolles in the graduate study of civil engineering (direction: hydrotechnics) at the University of Split, Faculty of Civil Engineering, Architecture and Geodesy. Graduated on 18. July 2014. under mentorship of Prof. dr. sc. Mijo Vranješ with the title: "Physical model RC permeable breakwater", and gained the title Master of science in civil engineering. From June 2015. to June 2016. has been employed as an apprentice at the Technical Service of Split Clinical Hospital Center. Later in 2016, starts as a Ph.D. Assistant at the Department of Technical Mechanics at the University of Split, Faculty of Civil Engineering, Architecture and Geodesy.

Participated as an PhD student in the scientific-research project: Groundwater flow modeling in karst aquifers (HRZZ-UIP-2013-11-8103) (2014-2018). As a co-author, he has an original scientific paper in a journal referenced in WoS and CC bases and has participated in five international scientific conferences.

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