ROUTING AND ACTION

MEMORANDUM

ROUTING

TO:(1) Mathematical Sciences Division (Myers, Joseph)

Report is available for review

(2) Proposal Files   Report No.:   Proposal Number: 65294-MA.11

DESCRIPTION OF MATERIAL

CONTRACT OR GRANT NUMBER: W911NF-14-1-0480

INSTITUTION: Clemson University

PRINCIPAL INVESTIGATOR: Leo Rebholz

TYPE REPORT: Final Report

DATE RECEIVED: 10/31/17 5:26PM

PERIOD COVERED: 8/1/14 12:00AM through 7/31/17 12:00AM

TITLE: Final Report: Long-term Stable Conservative Multiscale Methods for Vortex Flows

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ACTION TAKEN BY DIVISION

(x) Report has been reviewed for technical sufficiency and IS [x] IS NOT [ ] satisfactory.

(x) Material has been given an OPSEC review and it has been determined to be non sensitive and, except for manuscripts and progress reports, suitable for public release.

(x) Perfomance of the research effort was accomplished in a satisfactory manner and all other technical requirements have been fulfilled.

(x) Based upon my knowledge of the research project, I agree with the patent information disclosed.

Approved by SSL\JOSEPH.D.MYERS on 11/1/17 6:58AM

ARO FORM 36-E

REPORT DOCUMENTATION PAGE	Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY) 31-10-2017	2. REPORT TYPE Final Report	3. DATES COVERED (From - To) 1-Aug-2014 - 31-Jul-2017

4. TITLE AND SUBTITLE Final Report: Long-term Stable Conservative Multiscale Methods for Vortex Flows	5a. CONTRACT NUMBER W911NF-14-1-0480
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER 611102
6. AUTHORS	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES Clemson University 300 Brackett Hall Box 345702 Clemson, SC 29634 -5702	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	10. SPONSOR/MONITOR'S ACRONYM(S) ARO
	11. SPONSOR/MONITOR'S REPORT NUMBER(S) 65294-MA.11

12. DISTRIBUTION AVAILIBILITY STATEMENT

Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Leo Rebholz
UU	UU	UU	UU		19b. TELEPHONE NUMBER 864-656-1840

Standard Form 298 (Rev 8/98)
Prescribed by ANSI Std. Z39.18

RPPR Final Report
as of 01-Nov-2017

Agency Code:

Proposal Number: 65294MA **Agreement Number: W911NF-14-1-0480**

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Report Date: 31-Oct-2017 Date Received: 31-Oct-2017
Final Report for Period Beginning 01-Aug-2014 and Ending 31-Jul-2017
Title: Long-term Stable Conservative Multiscale Methods for Vortex Flows
Begin Performance Period: 01-Aug-2014 **End Performance Period:** 31-Jul-2017
Report Term: 0-Other
Submitted By: Leo Rebholz Email: rebholz@clemson.edu
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Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 3 **STEM Participants:** 6

Major Goals: To develop new, physically-motivated approaches for simulation of 3D incompressible vortical flows. Methods are expected to conform sharply to geometrical and physical structures, and the application of fundamental interest is the formation and evolution of wingtip vortices. The discretizations should base on variational multiscale principles, admit efficient algebraic solution strategies, and be amenable to numerical analysis. Presenting such analysis, as well as numerical validations, is also within the objectives.

Accomplishments: The numerical approach to accurate and long-term stable modelling of vortical flows developed within the project is based on several fundamental principles: (i) the discrete consistency to the geometric structure of the flow problem, evidenced through the balance laws for the array of Euler invariants; (ii) direct resolution of vector vorticity variable using the vorticity dynamic equation; (iii) stable splitting methods of velocity-vorticity coupled methods for time integration. Below we give details of the main results of the project.

A critical point in setting up numerical methods based on vorticity dynamics is defining suitable vorticity boundary conditions on solid wall boundaries. Setting these conditions correctly has been a long standing controversial question in CFD. Within this project, this question was addressed and the ultimate answer was found - a new vorticity boundary condition was derived from first principles, for the specific purpose of using it with the proposed vorticity-velocity method for solving the Navier-Stokes equations (NSE). The boundary condition is natural in the sense of variational PDE formulations, and hence can be implemented in numerical codes through the boundary integrals in a finite element method framework. This results in a vorticity boundary condition, which is efficient and likely much more accurate than commonly used ad-hoc methods. We found the direct relation between the derived condition and the latitude and longitude vorticity generation on solid walls streamlined by a fluid flow. This relation discovers the role of wall curvature in the intensification or suppression of the vorticity generation over the solid objects immersed in fluid flows. A paper was prepared that analyzes and tests this new boundary condition; it is published in "Computer Methods in Applied Mechanics and Engineering".

The developed natural vorticity boundary conditions allowed us to efficiently utilize vorticity dynamics equations in the numerical method and benefit from more physically consistent and accurate discrete vorticity. Following this paradigm, we proposed new schemes based on momentum, mass conservation and vorticity dynamics equations were studied. One key suggestion was to use the recovered discrete vorticity to drive nonlinear flow dynamics through the Lamb vector term in the momentum equation. We studied stability properties of the proposed vorticity-velocity schemes, and found that these scheme has better long-time stability properties than anything in the literature. More specifically, in the 2D case, both velocity and vorticity are L2 and H1 stable over long time, with constants having only polynomial dependence on the Reynolds number, and without a time step restriction. By contrast, common schemes in usual velocity-pressure form have time step restrictions for long-time stability, and constants with exponential dependence on the Reynolds number. This means that in 3D, one can be assured that instabilities in our proposed methods comes only from vortex stretching, which is where it should come from, and not from other sources related to discretization error. A paper was prepared that reports on this studies of the stability fluid flows numerical simulations. The paper is published in “Numerische Mathematik”.

Further, based on this numerical formulation we started the development of a multiscale method that should model the effect of unresolved vorticity and velocity subscales on the resolved scales. Since relatively little is known in the literature on the phenomenology of coarse—fine scale interaction in vorticity and hence the modeling of subgrid vorticity tensor, we took the residual-based Variational Multiscale (VMS) approach. In this approach, one defines large scales in terms of projections into appropriate functional spaces, and further, a system of equations for the coarse scales follows from a variational problem formulation and a set of explicitly formulated assumptions about the space decomposition and local properties of the involved operators. This joint work with the UofH PhD student Kyle Williams got interest of the DOE Office of science and Kyle was awarded DOE SCGSR award. Over the summer of 2017 we collaborated with Dr Pavel Bochev and his group from Sandia National Lab on this topic, and a paper resulting from this collaborative research is in preparation and should appear on arXiv in November 2017.

Continuing our effort to build cost-effective numerical methods based on reduced order modelling principle, we proposed, analyzed and tested a post-processing implementation of a projection based VMS method with proper orthogonal decomposition (POD) for the incompressible NSE. In this method, the projection-based VMS stabilization was added as a separate post-processing step to the standard POD approximation, and since the stabilization step is completely decoupled, the method can easily be incorporated into existing codes, and stabilization parameters can be tuned independent from the time evolution step. We were able analyze the method theoretically.   The method was applied to benchmark problems, and obtained numerical results both illustrate the theory and show the proposed method’s effectiveness. The paper is published in “Computer Methods in Applied Mechanics and Engineering”

Following the major objective of the project, we developed Galerkin discretizations, which conform sharply to geometrical structure of the NSE. This is one of the major goals of the project. To this end, we first studied conservation properties of Galerkin methods for the incompressible flow equations, without the divergence constraint strongly enforced. Note that in typical discretizations such as the mixed finite element method, the conservation of mass is enforced only weakly, and this leads to discrete solutions which may not conserve energy, momentum, angular momentum, helicity, or vorticity, even though the physics of the NSE dictate that they should. Next, we were looking for a discrete formulation that conserves as many physical laws as possible without utilizing a strong enforcement of the divergence constraint. This research leads us to an absolutely new formulation that conserves each of energy, momentum, angular momentum, enstrophy in 2D, helicity and vorticity (for reference, the usual Galerkin method in pressure-velocity variables and convective formulation does not conserve most of these quantities). We performed numerical studies, which verify the theory, tested the new formulation, and compared it to commonly used formulations. These studies showed the clear advantage of the new formulation in the Euler limit of the viscous fluid and very good performance for moderate Re numbers. The paper is published in “Journal of Computational Physics”

Significant progress was made on building efficient linear algebraic solvers for the saddle point linear systems arising in the developed schemes. Although developed as part of this project, these linear solvers are quite general and applicable to most any velocity-pressure NSE finite element code. Efficient and robust solvers are a crucial component for all incompressible flow simulation schemes. We developed improvements to commonly used algebraic splitting methods that allow for simpler Schur complement solves (the hard part of the solving the saddle point linear systems)- the Schur complements in the method are always symmetric positive definite, and do not change with the timestep. Such methods naturally introduce error, and our improvements (based on a reformulation) decrease the error by a full order of magnitude, i.e. O(\Delta t^3) instead of O(\Delta t^2). Our numerical tests showed that the error created by our method is smaller than the solver tolerances of the iterative solvers being used (in other words, error caused by the splitting method is negligible). This work was published in "SIAM Journal on Scientific Computing"

Training Opportunities: Several students were trained as part of this project:

PHD Completed
- Muhammad Mohebujjaman Ph.D. 2017, Clemson [now postdoc at Virginia Tech]

PHD In Progress
- Mengying Xiao, (PhD expected August 2018), Clemson
- Sergey Charnyi (PhD expected August 2018), Clemson
- Kyle Williams, (PhD expected 2018 or 2019), University of Houston
- Camille Zerfas, (PhD expected 2019), Clemson

MS Completed
- Camille Zerfas, MS May 2016, Clemson
- Rebecca Knoll, MS May 2016, Clemson
- Monica Morales Hernandez, MS August 2015, Clemson

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Results Dissemination: 10 papers about our results were published in the top tier journals of our field (SIAM journals, Journal of Computational Physics, Numerische Mathematik, Computer Methods in Applied Mechanics and Engineering).

Additionally, the PIs gave many talks about their work at many conferences and universities:

- M. A. Olshanskii, The 9th Workshop on Analysis and Advanced Numerical Methods for Partial Differential Equations (not only) for Junior Scientists" (July 4-8, 2016, Strobl, Austria
- M. A. Olshanskii, Third International conference on Super-computing technologies of mathematical modelling (Steklov Institute, Moscow, June, 2016)
- M. A. Olshanskii, European Congress on Computational and Applied Mathematics and Engeneering, Eccomas 2016 (Crete, June, 2016)
- M. A. Olshanskii, Scientific computing seminar of Math \& Sci Comp. Dept. at Emory (April 28, 2016)
- M. A. Olshanskii, 14th Copper Mountain conference on iterative methods (March 2016)
- M. A. Olshanskii, Center for Thermo-Fluid Mechanics of University of Houston (October 2017)
- M. A. Olshanskii , 9th International Conference on Finite Elements in Flow Problems, with a Keynote talk to minisymposium ``Stabilized, Multiscale, and Isogeometric Methods in CFD'' (Rome, April 2017)
- M. A. Olshanskii, 11th International Conference on ``Large-Scale Scientific Computations'' with invited talk to MS ``Advances in Heterogeneous Numerical Methods for Multi Physics Problems'' (Sozopol, Bulgaria, June 2017)
- M. A. Olshanskii, AMS Fall Western Sectional Meeting, with invited talk to ``Special Session on Above and Beyond Fluid Flow studies: In celebration of the 60th birthday of Prof. William Layton'' (Denver, CO, October 2016)

- L. Rebholz, 13th US National Congress on Computational Mechanics, SS on Old and New Challenges for Navier-Stokes Equations, San Diego CA (July 2015)
- L. Rebholz, Colloquium Talk, Matheamtical Sciences Department, Michigan Tech (September 2015)
- L. Rebholz, Fall 2015 Finite Element Circus, UMass Dartmouth (October 2015)
- L. Rebholz, Applied Math Seminar Talk, University of Alberta (October 2015)
- L. Rebholz, Colloquium Talk, Scientific Computing Department, Florida State (January 2016)
- L. Rebholz, SIAM Southeast 2016, Special session on Recent advances in fluid flow and applications, U. Georgia (March 2016)
- L. Rebholz, Conference on `Numerical Analysis and Predictability of Fluid Motion', University of Pittsburgh (May 2016)
- L. Rebholz, University of Tennessee, Department of Mathematics Colloquium, (September 2016)
- L. Rebholz, Tulane, Department of Mathematics Colloquium, (November 2016)
- L. Rebholz, Joint Math Meetings 2017, Special session on recent advances in numerical analysis of PDEs, Atlanta GA (January 2017)
- L. Rebholz, SIAM Computational Science and Engineering 2017, Special session on reduced order models for fluids, Atlanta GA (February 2017)
- L. Rebholz, Tenth IMACS Int. Conf. on Nonlinear Evolution Equations and Wave Phenomena, special session on Analysis of numerical methods for dispersive and fluid equations, Athens GA (March 2017)
- L. Rebholz, SIAM Annual 2017, SS on Synergy of Design, Analysis, and Computations in Fluid Flow Dynamics, Pittsburgh PA (July 2017)
- L. Rebholz, Mathematical Congress of the Americas 2017, SS on Equations of Fluid Mechanics: Numerics, Montreal CA (July 2017)
- L. Rebholz, Indiana University, Institute for Scientific Computing Seminar (January 2017)

Honors and Awards: Ph.D. student Kyle Williams won a DOE scholarship in 2017.

From the press release, "Kyle Williams is one of just 53 students in the nation chosen for the DOE’s Office of Science Graduate Student Research Program, and the only one working in applied mathematics."

Protocol Activity Status:

Technology Transfer: Dr. Chris Kees (Vicksburg Lab) was using the algebraic splitting methods we developed for his work in incompressible fluid flow simulation. To the best of our knowledge, he was using them in reservoir simulations, and had intern Alistair Bentley implementing them.

PARTICIPANTS:

Participant Type: Co PD/PI
Participant: Maxim Olshanskii
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Kyle Williams
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: PD/PI
Participant: Leo Rebholz
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Mengying Xiao
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Muhammad Mohebujjaman
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Camille Zerfas
Person Months Worked: 1.00 **Funding Support:**

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Sergey Charnyi
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Nothing to report in the uploaded pdf (see accomplishments)