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7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
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PO Box 751 (SPA)

Portland, OR 97207 -0751

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INVESTIGATOR(S):

Name: Panayot Vassilevski
Email: panayot@pdx.edu
Phone Number: 5037253292
Principal: Y

Organization: **Portland State University**
Address: PO Box 751 (SPA), Portland, OR 972070751
Country: USA

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Phone: (503) 725-3292
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Major Goals: Many simulations in science and engineering described by partial differential equations demand the use of
powerful computational resources and rely on efficient software libraries that can utilize these resources. With the ever increase of data and need for better accuracy in the simulations for processes that evolve in time, the efficient use of computer resources reaches a point when one can take benefit of increased number of parallel processors if the simulations are performed in the combined space-time domain. The latter is challenging since it increases the memory requirement by an order of magnitude since a simulation formulated in a 3D physical space domain has to be run now in a 4D combined space-time domain. The project aims to alleviate this severe memory constraint by developing new discretization techniques in combined space-time domain that utilize dimension reduction which is accurate enough and lead to discrete problems that can be efficiently solved by existing parallel software libraries that are designed to work independently of the dimension of the problem. The above goals can be achieved in two complementary ways: one, by designing efficient adaptive mesh refinement (AMR) discretization procedures in the combined space-time computational domain, and then applying dimension reduction to further achieve memory savings. All this is possible after efficient scalable mesh generation and construction of classes of space-time (4D) finite elements are designed, analyzed and made available in scalable libraries. This was the main corner-stone goal of the project.

Accomplishments: Key accomplishments:

(i) A main accomplishment: We designed finite element spaces for the whole de Rham sequence in 4D. The 4D finite element spaces are the first ones ever designed that are made publicly available to the research community; they are
accessible through the public finite element library MFEM, mfem.org and also through the library [1].

(ii) The 4D finite element spaces have been extensively tested
in terms of approximation properties with results documented in [2]..

(iii) We have designed and implemented a parallel domain decomposition type solver for a broad class of CFOSLS discretized problems with divergence type constraint that typically arises for conservation equations discretzied in space-time domain. The solver is available through our publicly accessible code [1].

(iv) We have designed, analyzed and tested a large class of scalable preconditioners for the main canonical bilinear forms associated with the 4D de Rham sequence. The results are summarized in a publication [3]. These preconditioners are needed as building tools for the problems of our main interest such as the first order system least-squares with conservation constraints (CFOSLS) applied to time-dependent PDEs (partial differential equations) including transport (conservation law) equations.

References
[1] K. Voronin and P.S. Vassilevski, "A domain decomposition divergence-free solver for CFOSLS discretized conservation equations". https://github.com/CFOSLS.

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"Space-Time Discretizations Using Constrained First-Order System Least-Squares (CFOSLS)", Journal of Computational Physics (2018), https://doi.org/10.1016/j.jcp.2018.07.024.

[3] J. Gopalakrishnan, M. Neumueller, and P. S. Vassilevski,
"{\em The auxiliary space preconditioner for the de Rham complex,}" SIAM Journal on Numerical Analysis (to appear). Available at http://web.pdx.edu/~gjay/pub/hx.pdf .

Training Opportunities: A main training opportunity was the participation of the postdoc Kirill Voronin.
His gained exposure and became expert and main collaborator of the PI, on a variety of topics by overcoming substantial amount of technical and high volume material, which involved:
(i) The further development of the new finite element discretization technique (CFOSLS - First Order System Least Squares with constraints) applied to time-dependent problems.
(ii) The construction of new 4D (space-time) conforming finite elements; their parallel implementation and use to build CFOSLS type discretization schemes for classes of time-dependent PDEs (partial differential equations).
(iii) learned and became regular user of sophisticated highly scalable parallel libraries: MFEM - finite elements, and HYPRE - scalable preconditioners, both developed at LLNL (Lawrence Livermore National Laboratory).
(iv) Designed, analyzed, implemented and tested sophisticated geometric multilevel domain decomposition solver for CFOSLS type discretization problems with divergence constraint, which cover conservation law (transport) equations in space-time domain.
(v) Co-authored with a leading role of a major journal publication on the project work.

Results Dissemination: The results were presented in several publications with a release of a software library for the main studied project topic CFOSLS: "Constrained First Order Systems Least Squares".

Honors and Awards: During the last year of the project the PI was named a SIAM (Society for Industrial and Applied Mathematics) fellow class of 2018 for his research and scholarship.

Protocol Activity Status:

Technology Transfer: We released the produced by the project CFOSLS discretization and solvers software for public use and further development:

https:\\github.com/CFOSLS : "CFOSLS: a domain decomposition divergence-free solver for CFOSLS discretized conservation equations".

PARTICIPANTS:

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

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)

Participant: Kirill Voronin
Person Months Worked: 15.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
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Other Collaborators:

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Date Received: 28-Aug-2017 Conference Date: 06-Jul-2016 Date Published: 10-Jul-2016
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Paper Title: Space-time CFOSLS methods with AMGe upscaling
Authors: Martin Neumueller, Panayot S. Vassilevski, and Umberto Villa
Acknowledged Federal Support: **Y**

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Conference Location: Jeju Island, Korea
Paper Title: Parallel Solver for H(div) Problems Using Hybridization and AMG
Authors: Chak S. Lee, Panayot S. Vassilevski
Acknowledged Federal Support: **Y**

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Authors: Chak S. Lee, Panayot S. Vassilevski
Acknowledged Federal Support: **Y**

WEBSITES:

URL: https://github.com/CFOSLS/
Date Received: 07-Sep-2018
Title: CFOSLS: a domain decomposition divergence-free solver for CFOSLS discretized conservation equations
Description: We have designed and implemented a parallel domain decomposition type solver for a broad class of CFOSLS discretized problems with divergence type constraint that typically arises for conservation equations discretzied in space-time domain. The solver is publicly available at this web site. Its performance is documented in the publication: K. Voronin, C.S. Lee, M. Neumueller, P. Sepulveda, and P. S. Vassilevski, "Space-Time Discretizations Using Constrained First-Order System Least-Squares (CFOSLS)", Journal of Computational Physics 373(2018), pp.~863-876. https://doi.org/10.1016/j.jcp.2018.07.024.

RPPR Final Report
as of 10-Oct-2018

FINAL REPORT: ARO GRANT W911NF1510590
SECTION 3.4 NUMERICAL ANALYSIS
SPACE-TIME DISCRETIZATIONS ENABLING PARALLEL-IN-TIME SIMULATIONS

PANAYOT S. VASSILEVSKI (PI)

Abstract. This is the final report of a computational research project funded by ARO on constrained least-squares finite element discretizations of classes of PDEs (partial differential equations) in combined space-time domain. More specifically, we study least-squares finite elements applied to PDEs rewritten as first order systems in terms of derivatives and posed as a minimization of a least-squares functional. The minimization functional is subject to a constraint to maintain conservation. We outline the main accomplishments and a possible venue for continuation to achieve the ultimate goal; namely, to derive discretizations that are best adapted to follow the physics modeled by the underlined PDE, and compare them with the more traditional state-of-the art time-stepping schemes, both in terms of accuracy and parallel scalability.

1. Project objectives: major goals

Many simulations in science and engineering described by partial differential equations demand the use of powerful computational resources and rely on efficient software libraries that can utilize these resources. With the ever increase of data and need for better accuracy in the simulations for processes that evolve in time, the efficient use of computer resources reaches a point when one can take benefit of increased number of parallel processors if the simulations are performed in the combined space-time domain, i.e., utilizing one extra dimension. The latter is challenging since it increases the memory requirement by an order of magnitude since a simulation formulated in a 3D physical space domain has to be run now in a 4D combined space-time domain. The project aims to alleviate this severe memory constraint by developing new discretization techniques in combined space-time domain that utilize dimension reduction which is accurate enough and lead to discrete problems that can be efficiently solved by existing parallel software libraries that are designed to work independently of the dimension of the problem.

2. Accomplishments

(i) A main accomplishment: We designed finite element spaces for the whole de Rham sequence in 4D. The 4D finite element spaces are the first ones ever designed that are made publicly available to the research community; they

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1991 *Mathematics Subject Classification.* 65F10, 65N20, 65N30.
Key words and phrases. least squares finite elements, local refinement.

are accessible through the public finite element library MFEM, mfem.org and also through the library [CFOSLSlib].

(ii) The 4D finite element spaces have been extensively tested in terms of approximation properties with results documented in [Vo18].

(iii) We have designed and implemented a parallel domain decomposition type solver for a broad class of CFOSLS discretized problems with divergence type constraint that typically arise for conservation equations discretzied in space-time domain. The solver is available through our publicly accessible code [CFOSLSlib].

(iv) We have designed, analyzed and tested a large class of scalable preconditioners for the main canonical bilinear forms associated with the 4D de Rham sequence. The results are summarized in a publication to appear, [GNV]. These preconditioners are needed as building tools for the problems of our main interest such as the first order system least-squares with conservation constraints (CFOSLS) applied to time-dependent PDEs (partial differential equations) including transport (conservation law) equations.

(v) We have performed first comparison tests between state-of-the-art time stepping procedures and multilevel solvers for our space-time CFOSLS discretization schemes (for details, see Section 3.1), which demonstrated the potential of the combined space-time discretizations to be more competitive in terms of time-to solution at large scale.

3. Preliminary comparison tests and future directions

With the current funding cycle, the ultimate objective to compare state-of-the-art parallel-in-time solvers exploiting more traditional time-stepping discretization schemes with solvers for the newly designed CFOSLS schemes in the combined space-time domain was only preliminary tested for a number of reasons. First, the 4D elements, their implementation in a scalable finite element library as well as the design of scalable preconditioners for the building blocks of the 4D de Rham complex ([GNV]) took substantial amount of time. Never-the-less the proposed CFOSLS discretizations in 4D accompanied with a general parallel multilevel domain decomposition solver were completed in time with a publication [Vo18] and with a corresponding code release found in [CFOSLSlib]. More over, our preliminary comparison test (described below) between traditional time-stepping discretization schemes and our CFOSLS discretization showed that utilizing more processors can lead to faster performance of multigrid solvers applied to the CFOSLS discretization than using state-of-the-art solvers at every time-step in a traditional backward Euler time-stepping scheme. The details are given below.

3.1. Strong scaling comparison results.

We consider the heat equation

$$\partial_t S - \mathrm{div}_{\mathbf{x}}\big(\nabla S\big) = f(x,t), \qquad \text{for all } (x,t) \in \Omega_T. \tag{3.1}$$

The space-time domain Ω_T is $(0,1)^4$, and the exact solution is given by

$$u(\mathbf{x},t) = t^2 e^t \prod_{i=0}^{2} \sin\Big((3-i)\pi x_i\Big).$$

The right-hand side f in (3.1) is computed using the exact u.

We are interested in comparing traditional time stepping scheme versus space-time discretization using the developed by this project combined space-time CFOSLS discretization method.

To get as close as possible to "*apple-to-apple*" comparison, we use the same mesh for both discretization schemes. Also, in the traditional time-stepping method, we use at every time step a mixed finite element discretization, since it provides approximation to both S and its gradient, which is comparable to the CFOSLS scheme (also providing approximations to S and its gradient). The mesh is generated by an initial unstructured simplicial 3D mesh, which we refine to generate larger problems, and the total numbers of degrees of freedom are shown in Table 2. For the time-stepping method, the total numbers of degrees of freedom is the problem size in each time step multiplied by the number of time steps.

TABLE 1. Number of elements

refinement level	3D (tetrahedron)	4D (pentatope)
1	6,851	393,216
2	54,808	6,291,456
3	438,464	100,663,296

TABLE 2. Total number of dofs (unknowns) of different methods

refinement level	3D (time-stepping)	4D (CFOSLS)
1	1,222,284	1,421,857
2	20,568,184	22,513,729
3	342,847,120	358,359,169

For the time-stepping method, we discretize in space using mixed finite elements (Raviart-Thomas elements - RT0 + P0) in 3D, and backward Euler for time-stepping scheme. In each time step, the saddle point system is solved using the state-of-the-art solvers, namely the hybridization one (from [LV17]) combined with the BoomerAMG (algebraic multigrid) from the LLNL hypre library.

The 4D mesh is generated based on the 3D mesh by embedding as described in detail in [KV18]. In CFOSLS, three finite element spaces in 4D are used ($H(\text{div})$, H^1 and L^2). The 3-by-3 block system is solved by divergence-free solver, in which we find a particular solution using a multilevel algorithm, and then restrict to system to a divergence free subspace and solve by monolithic geometric multigrid. The details are found in our paper [Vo18]. The number of (MG) levels is the same as the refinement levels (see Table 2). The smoother in the monolithic multigrid is lower triangular block smoother, with each diagonal block being the scalar ℓ_1 Gauss-Seidel smoother of the block. The coarse solver is block diagonal smoother (with ℓ_1 Gauss-Seidel in each block), the tolerance of the coarse solver is the same as the overall MG solver, with max number of iteration set to 10.

In both solution methods, the relative and absolute tolerance for the linear solvers are set to 1e-6 and 1e-7 respectively.

TABLE 3. Strong scaling - time-stepping

#proc	Total time-stepping time
30	39.75s
60	24.35s
120	16.9s
250	13.67s
500	13.09s
1000	13.67s
2000	14.75s
3600	14.98s

TABLE 4. Strong scaling - CFOSLS

#proc	Total CFOSLS solving time (#iter)
120	104.54s (53)
500	29.36s (58)
1000	17.38s (60)
2000	12.59s (65)
3600	9.35s (65)

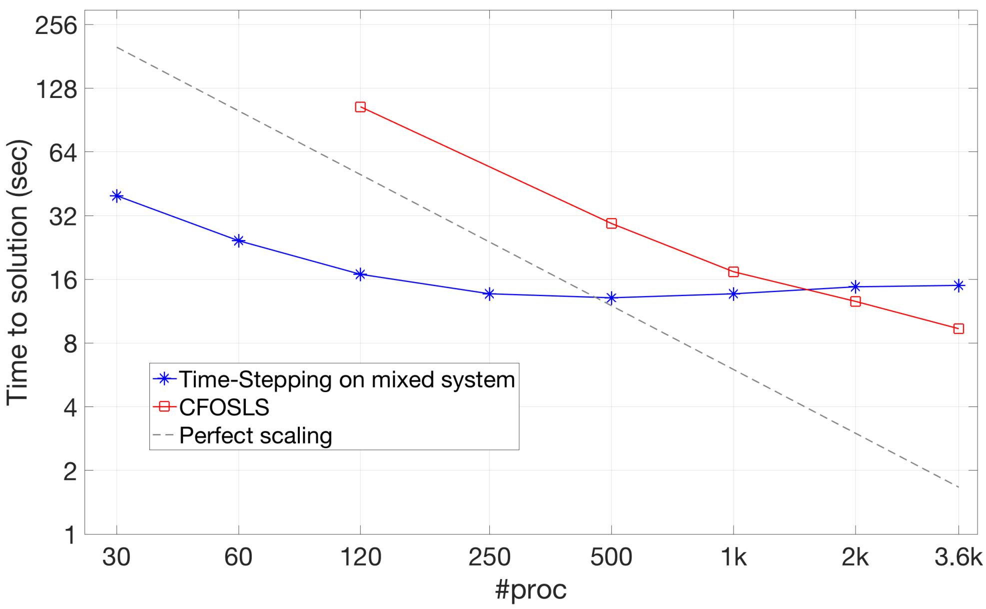

FIGURE 1. Strong scaling comparison . The tests were run on LLNL cluster Quartz, cf., https://hpc.llnl.gov/hardware/platforms/Quartz

It is clear from Figure 1, that adding more processors leads to faster saturation in time-to-solution in the traditional time-stepping scheme, whereas in the CFOSLS discretization, it continues to be beneficial much longer and leads to overall faster method for this test example. All this is in agreement with the currently existing parallel-in-time solvers, namely, that more processors can lead to overall faster solution than using the same (large) number of processors in traditional time-stepping approaches.

3.2. **Concluding remarks.** We stress upon the fact that presented research is typically performed in a national laboratory by a team of researchers. In our case, the project funded the PI, a full time postdoc and short visits by our main collaborator M. Neumueller from University of Linz, Austria. We did also leverage some collaborative work with researchers from LLNL. A main obstacle for performing more thorough (and fair) solvers comparison is the need for AMR (adaptive mesh refinement) in combined space-time domain. This is what we consider a natural possible continuation step of the performed space-time research.

More specifically, to complete the study in terms of comparison of scalable (state-of-the-art) solvers built for more traditional time-stepping discretizations versus solvers for the combined 4D space-time discretizations, for fair comparison we need the 4D discretization to be produced in a (some sense) optimal way, e.g., by utilizing AMR in 4D. Such a discretization strategy has the potential to alleviate for example any CFL time-stepping conditions (since there will be no clear time-stepping direction). Once such an AMR based CFOSLS discretization is derived, for possible further memory reduction, we can employ the originally proposed element agglomeration based upscaling technique which showed great potential in our preliminary tests in 3D (two space plus time) dimensions, cf. [NVV].

We stress upon the fact that 4D AMR is a project on its own. Although there are several algorithms available to produce local element refinement in any D, there are none actually implemented in 4D that are publicly available in a scalable (distributed) parallel library. Also, there is a need for some theoretical study for CFOSLS AMR strategies in 4D as well, in particular designing an adequate adaptive finite element procedures and proving their convergence. We have started some preliminary studies in that direction, cf. [HKV], for plain FOSLS, and in [CFOSLSlib] for CFOSLS. We note however that the well established AFEM recipes (cf., e.g., the popular lecture note [AFEM]) for elliptic PDEs, do not seem to translate in any straightforward way even to plain discretization schemes of FOSLS type (i.e. without constraints), so some new research is of potential interest here.

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[GNV] J. Gopalakrishnan, M. Neumueller, and P. S. Vassilevski, "*The auxiliary space preconditioner for the de Rham complex,*" SIAM J. Numer. Anal. (to appear). Available at http://web.pdx.edu/~gjay/pub/hx.pdf

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Fariborz Maseeh Depratment of Mathematics and Statistics, Portland State University, PO Box 751, Portland, OR 97207, U.S.A.

Email address: panayot@pdx.edu