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Open Science Philosophy

Open science encompasses unrestricted access to scientific research articles, access to data from public research, and collaborative research enabled by information and communication technology tools, models, and incentives. Broadening access to scientific research publications and data is at the heart of open science. The objective of open science is to make research outputs and its potential benefits available to the entire world and in the hands of as many as possible:

- Open science promotes a more accurate verification of scientific research results. Scientific inquiry and discovery can be sped up by combining the tools of science and information technologies. Open science will benefit society and researchers by providing faster, easier, and more efficient availability of research outputs.
- Open science reduces duplication in collecting, creating, transferring, and re-using scientific material.
- Open science increases productivity in an era of tight budgets.
- Open science results in great innovation potential and increased consumer choice from public research.
- Open science promotes public trust in science. Greater citizen engagement leads to active participation in scientific experiments and data collection.

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Open Society

An open society allows individuals to change their roles and to benefit from corresponding changes in status. Open science depends to a greater or lesser extent on digital technologies and innovations in structural processes by an open society. When realized, open science research and innovation can create investment opportunities for new and better products and services and therefore increase competitiveness and employment. Open science research and innovation is a key component of thematic open science priorities. Central to the open science digital infrastructure is enabling industry to benefit from digital technology and to underpin scientific advances through the development of an open society. Open science research and innovation can also contribute to society as a global actor because scientific relations can flourish even where global relations are strained. Open science has a critical role across many areas of decision making in providing evidence that helps understand the risks and benefits of different open science choices. Digital technology is making the conduct of open science and innovation more collaborative, more global, and more open to global citizens. Open society must embrace these changes and reinforce its position as the leading power for science, for new ideas, and for investing sustainably in the future.

It is apparent in open society that the way science works is fundamentally changing, and an equally significant transformation is taking place in how organizations and societies innovate. The advent of digital technology is making research and innovation more open, collaborative, and global. These exchanges are leading open society to develop open science and to set goals for research and innovation priority. Open science goals are materializing in the development of scientific research and innovation platforms and greater acceptance of scientific data generated by open science research. Open science research and innovation do not need help from open society to come up with great ideas, but the level of success ideas ultimately reach is undoubtedly influenced by regulation, financing, public support, and market access. Open society is playing a crucial role in improving all these success factors.

Open Science

Open science represents a new approach to the scientific process based on cooperative work and new ways of diffusing knowledge by using digital technologies and collaborative tools. These innovations capture a systemic change to the way science and research have been carried out for the last fifty years. Science is shifting from the standard practice of publishing research results in scientific publications after the research and reviews are completed. The shift is towards sharing and using all available knowledge at an earlier stage in the research process. Open science is to science what digital technology is to social and economic transactions: allowing end users to be producers of ideas, relations, and services and in doing so, enabling new working models, new social relationships and leading to a new modus operandi for science. Open science is as important and disruptive as e-commerce has been for the retail industry. Just like e-commerce, the open science research paradigm shift affects the whole business cycle of doing science and research. From the selection of research subjects to the carrying out of research, to its use and re-use, to the role of universities, and that of publishers are all dramatically changed. Just as the internet and globalization have profoundly changed the way we do business, interact socially, consume culture, and buy goods, these changes are now profoundly impacting how one does research and science.

The discussion on broadening the footprint of science and on novel ways to produce and spread knowledge gradually evolved from two global trends: Open Access and Open Source. The former refers to online, peer-reviewed scholarly outputs, which are free to read, with limited or no copyright and licensing restrictions, while open source refers to software created without any proprietary restriction and which can be accessed and freely used. Although open access became primarily associated with a particular publishing

or scientific dissemination practice, open access already sought to induce a broader practice that includes the general re-use of all kinds of research products, not just publications or data. It is only more recently that open science has coalesced into the concept of a transformed scientific practice, shifting the focus of researchers' activity from publishing as fast as possible to sharing knowledge as early as possible. Open science is defined as the idea that scientific knowledge of all kinds should be openly shared as early as is practical in the discovery process. As a result, the way science is done in the future will look significantly different from the way it is done now. Open science is the ongoing evolution in the modus operandi of doing research and organizing science. This evolution is enabled by digital technology and is driven by both the globalization of the scientific community and increasing public demand to address the societal challenges of our times. Open science entails the ongoing transitions in the way research is performed, researchers collaborate, knowledge is shared, and science is organized.

Open science impacts the entire research cycle, from the inception of research to its publication, and on how this cycle is organized. The outer circle reflects the new interconnected nature of open science, while the inner circle shows the entire scientific process, from the conceptualization of research ideas to publishing. Each step in the scientific process is linked to ongoing changes brought about by open science, including the emergence of alternative systems to establish a scientific reputation; changes in the way quality and impact of research are evaluated; the growing use of scientific blogs; open annotation; and open access to data and publications. All institutions involved in science are affected, including research organizations, research councils, and funding bodies. The trends are irreversible, and they have already grown well beyond individual projects. Theses changes predominantly result from a bottom-up process driven by a growing number of researchers who increasingly employ social media in their research and initiate globally coordinated research projects while sharing results at an early stage in the research process.

Open science is encompassed in five schools of thought:

- o the infrastructure school, concerned with technological architecture
- o the public school, concerned with the accessibility of knowledge creation
- the measurement school, concerned with alternative impact assessment
- o the democratic school, concerned with access to knowledge
- o the pragmatic school, concerned with collaborative research

According to the measurement school, the reputation and evaluation of individual researchers are still mainly based on citation-based metrics. The h-index is an author-level metric that attempts to measure both the productivity and citation impact of the publications of a scientist or scholar. The impact factor is a measure reflecting the average number of citations to articles published in an academic journal and is used as a proxy for the relative importance of a journal.

Numerous criticisms have been made of citation-based metrics, primarily when used, and often misused, to assess the performance of individual researchers. These metrics:

- o are often not applicable at the individual level
- o do not take into account the broader social and economic function of scientific research
- o are not adapted to the increased scale of research
- o cannot recognize new types of work that researchers are performing

Web-based metrics for measuring research output, popularized as altmetrics, have recently received much attention: some measure the impact at the article level, others make it possible to assess the many outcomes of research in addition to the number of scientific articles and references. The current reputation and evaluation system has to adapt to the new dynamics of open science and acknowledge and incentivize

engagement in open science. Researchers engaging in open science have growing expectations that their work, including intermediate products such as research data, will be better rewarded or taken into account in their career development. Vice-versa, the use, and reuse of open data will require appropriate codes of conduct requiring, for example, the proper acknowledgment of the original creator of the data.

These ongoing changes are progressively transforming scientific practices with innovative tools to facilitate communication, collaboration, and data analysis. Researchers that increasingly work together to create knowledge can employ online tools and create a shared space where creative conversation and collaboration can occur. As a result, the problem-solving process can be faster, and the range of problems that can be solved can be expanded. The ecosystem underpinning open science is evolving very rapidly. Social network platforms for researchers already attract millions of users and are being used to begin and validate more research projects.

Furthermore, the trends towards open access are redefining the framework conditions for science and thus have an impact on how open innovation is produced by encouraging a more dynamic circulation of knowledge. It can enable more science-based startups to emerge thanks to the exploitation of openly accessible research results. Open science, however, does not mean free science. It is essential to ensure that intellectual property is protected before making knowledge publicly available in order to subsequently attract investments that can help translate research results into innovation. If this is taken into account, fuller and broader access to scientific publications and research data can help to accelerate innovation. Investments that boost research and innovation in open science would benefit society with fewer barriers to knowledge transfer, open access to scientific research, and greater mobility of researchers. In this context, open access can help overcome the barriers that innovative organizations face in accessing the results of research funded by the public.

Open innovation

An open society is the largest producer of knowledge, but the phenomenon of open science is changing every aspect of the scientific method by becoming more open, inclusive, and interdisciplinary. Ensuring open society is at the forefront of open science means promoting open access to scientific data and publications alongside the highest standards of research integrity. There are few forces in this globe as engaging and unifying as science. The universal language of science maintains open channels of communication globally. Open society can maximize its gains through maintaining its presence at the highest level of scientific endeavor, and by promoting a competitive edge in the knowledge society of the information age. The ideas and initiatives described in this publication can stimulate anyone interested in open science research and innovation. It is designed to encourage debate and lead to new ideas on what and open society should do, should not do, or do differently.

An open society can lead to a research powerhouse; however, open society rarely succeeds in turning research into innovation and in getting research results to the global market. Open society must improve at making the most of its innovation talent, and that is where open innovation comes into play. The basic premise of open innovation is to open up the innovation process to all active players so that knowledge can circulate more freely and be transformed into products and services that create new markets while fostering a stronger culture of entrepreneurship. Open innovation is defined as the use of purposive inflows and outflows of knowledge to accelerate internal innovation. This original notion of open innovation was primarily based on transferring knowledge, expertise, and even resources from one company or research institution to another. This notion assumes that firms can and should use external ideas as well as internal ideas, and internal and external paths to market, as they seek to improve their performance. The concept of open innovation is continually evolving and is moving from linear, bilateral transactions and collaborations

towards dynamic, networked, multi-collaborative innovation ecosystems. This means that a specific innovation can no longer be seen as the result of predefined and isolated innovation activities but rather as the outcome of a complex co-creation process involving knowledge flows across the entire economic and social environment. This co-creation takes place in different parts of the innovation ecosystem and requires knowledge exchange and absorptive capacities from all the actors involved, whether businesses, academia, financial institutions, public authorities, or citizens.

Open innovation is a broad term, which encompasses several different nuances and approaches. Two main elements underpin the most recent conceptions of open innovation: the users are in the spotlight and invention becomes an innovation only if users become a part of the value creation process. Notions such as user innovation emphasize the role of citizens and users in the innovation processes as distributed' sources of knowledge. This kind of public engagement is one of the aims of open science research and innovation. The term 'open' in these contexts has also been used as a synonym for 'user-centric'; creating a wellfunctioning ecosystem that allows co-creation and becomes essential for open innovation. In this ecosystem, relevant stakeholders are collaborating along and across industry and sector-specific value chains to cocreate solutions for socio-economic and business challenges. One important element to keep in mind when discussing open innovation is that it cannot be defined in absolutely precise terms. It may be better to think of it as a point on a continuum where there is a range of context-dependent innovation activities at different stages, from research to development through to commercialization, and where some activities are more open than others. Open innovation is gaining momentum thanks to new large-scale trends such as digitalization and the mass participation and collaboration in innovation that it enables. The speed and scale of digitalization are accelerating and transforming the way one designs, develops, and manufactures products, the way one delivers services, and the products and services themselves. It is enabling innovative processes and new ways of doing business, introducing new cross-sector value chains and infrastructures.

Open society must ensure that it capitalizes on the benefits that these developments promise for citizens in terms of tackling societal challenges and boosting business and industry. Drawing on these trends, and with the aim of helping build an open innovation ecosystem in open society, the open society's concept of open innovation is characterized by:

- o combining the power of ideas and knowledge from different actors to co-create new products and find solutions to societal needs
- o creating shared economic and social value, including a citizen and user-centric approach
- o capitalizing on the implications of trends such as digitalization, mass participation, and collaboration

In order to encourage the transition from linear knowledge transfer towards more dynamic knowledge circulation, experts agree that it is essential to create and support an open innovation ecosystem that facilitates the translation of knowledge into socio-economic value. In addition to the formal supply-side elements such as research skills, excellent science, funding and intellectual property management, there is also a need to concentrate on the demand side aspects of knowledge circulation, making sure that scientific work corresponds to the needs of the users and that knowledge is findable, accessible, interpretable and reusable. Open access to research results aims to make science more reliable, efficient, and responsive and is the springboard for increased innovation opportunities, e.g. by enabling more science-based startups to emerge. Prioritizing open science does not, however, automatically ensure that research results and scientific knowledge are commercialized or transformed into socio-economic value. In order for this to happen, open innovation must help to connect and exploit the results of open science and facilitate the faster translation of discoveries into societal use and economic value.

Collaborations with global partners represent important sources of knowledge circulation. The globalization of research and innovation is not a new phenomenon, but it has intensified in the last decade, particularly in terms of collaborative research, international technology production, and worldwide mobility of researchers and innovative entrepreneurs. Global collaboration plays a significant role both in improving the competitiveness of open innovation ecosystems and in fostering new knowledge production worldwide. It ensures access to a broader set of competencies, resources, and skills wherever they are located, and it yields positive impacts in terms of scientific quality and research results. Collaboration enables global standard-setting, allows global challenges to be tackled more effectively, and facilitates participation in global value chains and new and emerging markets.

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The scholarly research review is a multidimensional evaluation procedure in which standard peer review models can be adapted in line with the ethos of scientific research, including accessible identities between reviewer and author, publishing review reports and enabling greater participation in the peer review process. Scholarly research review methods are employed to maintain standards of quality, improve performance, provide credibility, and determine suitability for publication. *Responsible Peer Review Procedure:* Responsible peer review ensures that scholarly research meets accepted disciplinary standards and ensures the dissemination of only relevant findings, free from bias, unwarranted claims, and unacceptable interpretations. Principles of responsible peer review:

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- Scholarly Research Review Final-version Reviewing: Editorial revision of the language and format is conducted on the final version of the manuscript for publication
- Scholarly Research Review Platforms: The scholarly research review process is independent of the final publication of the manuscript and it is facilitated by a different organizational entity than the venue of publication

All submitted manuscripts are subject to the scholarly research review process, in which there are three stages of evaluation for consideration: pre-review manuscripts, chair-review presentation, and final-review manuscripts. All submitted full text papers, that may still be withstand the editorial review process, are presented in the conference proceedings. Manuscripts are tracked and all actions are logged by internal and external reviewers according to publication policy. External reviewers' editorial analysis consists of the evaluation reports of the conference session chairs and participants in addition to online internal and external reviewers' reports. Based on completion of the scholarly research review process, those manuscripts meeting the publication standards are published 10 days after the event date.

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TABLE OF CONTENTS

1	Preparation of Copper Manganese Oxide/Graphene Quantum Dot Nanocomposites for Supercapacitors Mohammad Ashourdan	1
2	Influence of Magnetized Water on the Split Tensile Strength of Concrete Justine Cyril E. Nunag, Nestor B. Sabado Jr., Jienne Chester M. Tolosa	27
3	Parallel Pipelined Conjugate Gradient Algorithm on Heterogeneous Platforms Sergey Kopysov, Nikita Nedozhogin, Leonid Tonkov	32
4	A 5G Architecture Based to Dynamic Vehicular Clustering Enhancing VoD Services Over Vehicular Ad hoc Networks <i>Lamaa Sellami, Bechir Alaya</i>	40
5	Enhanced Bit Error Rate in Visible Light Communication: A New LED Hexagonal Array Distribution Karim Matter, Heba Fayed, Ahmed Abd-Elaziz, Moustafa Hussein	46
6	Governance Challenges for the Management of Water Resources in Agriculture: The Italian Way Silvia Baralla, Raffaella Zucaro, Romina Lorenzetti	53
7	In vitro Skin Model for Enhanced Testing of Antimicrobial Textiles Steven Arcidiacono	54
8	Diagenesis and Depositional Facies Impact of Diagenetic Alterations on Reservoir Quality Evolution of Fluvial Sandstones, Nubian Formation, Sirt Basin, Northern Libya Faraj M. Elkhari	55
9	2D Modeling of Rockfall and Mitigation Measures on Roadcut Slopes Along Brgy. Mayong, Tiwi, Albay, Bicol Rose Razel Roman and Federico dela Peña	56
10	Study on Shifting Properties of CVT Rubber V-belt Natsuki Tsuda, Kiyotaka Obunai, Kazuya Okubo, Hideyuki Tashiro, Yoshinori Yamaji, Hideyuki Kato	73
11	On a Recursive Expansion to the Floor Function Mhatre Aatmaj Kaustubh	78
12	Strategic Interventions to Combat Socio-economic Impacts of Drought in Thar - A Case Study of Nagarparkar Anila Hayat	79
13	Continuous Land Cover Change Detection in Subtropical Thicket Ecosystems Craig Mahlasi	80
14	Lateral Torsional Buckling: Tests on Glued Laminated Timber Beams Vera Wilden, Benno Hoffmeister, Markus Feldmann	81
15	Implementation of Asynchronous SSVEP Brain Control System Using Riemannian Classifiers for Assistive Mobility Systems Prasanna Kolar, Mohammad Jamshidi	82
16	Low Density Parity Check Codes HAKIM LAHOUALI	94
17	Blue Economy and Marine Mining Fani Sakellariadou	95
18	Need for organic growing protocol for medicinal herbs satish kumar dhar	96
19	The Insecticidal Activity of Three Essential Oils on the Chickpea Weevil Callosobruchus Maculatus F (Coleoptera; Curculionidae) Azzaz Siham	97

20	In Vitro Digestibility of Grains and Straw of Seventeen Ecotypes of Bitter Vetch (Vicia ervilia) in the North of Morocco Boukrouh Soumaya, Cabaraux Jean-François, Avril Claire, Noutfia Ali, Chentouf Mouad	98
21	Sunil Gangopaddhaya's 'An Unsent Letter': A Harrowing Outburst of Long Smothered Wail of a Lacerated Psyche Mohammad Mozammel Haque	99
22	Does Explicit Knowledge Enhance Statistical Learning in Children with Language Development Disorder? Insights from ERPs Ana Paula Soares, Alexandrina Lages, Helena Oliveira, Francisco-Javier Gutiérrez-Domínguez, Marisa Lousada	100
23	Pricing Efficiency of Convertible Bonds in China Hao Zhang	101
24	Gender Discrimination in Elementary and High School in Croatia Based on a Students Research Ivana Šalinović	109
25	Academic Freedom Policy: A Case Study Marlin Killen	128
26	ECONOMÍA POLÍTICA HOY. Una perspectiva desde la espiritualidad Pedro José Morales Rodriguez	129
27	Open Bankins as an Instrumentof the Credit Access in Brazil Maylin Maffini	130
28	Social Anxiety Connection with Individual Characteristics: Theory of Mind, Verbal Irony Comprehension and Personal Traits Anano Tenieshvili, Teona Lodia	131
29	Social Anxiety Connection with Individual Characteristics: Theory of Mind, Verbal Irony Comprehension and Personal Traits Anano Tenieshvili, Teona Lodia	132
30	Acceptance and Commitment Therapy for Social Anxiety Disorder in Adolescence: A Manualized Online Approach Francisca Alves, Diana Figueiredo, Paula Vagos, Luiza Lima, Maria do Céu Salvador, Daniel Rijo	133
31	The Role of Self-Compassion for the Diagnosis of Social Anxiety Disorder in Adolescents Diana Vieira Figueiredo, Rita Ramos Miguel, Maria do Céu Salvador, Luiza Nobre-Lima, Daniel RIjo, Paula Vagos	134
32	The Breast Surgery Movement: A 50 Year Development of the Surgical Specialty Lauren Zammerilla Westcott, Ronald C. Jones, James W. Fleshman	135
33	Neuro-Epigenetic Changes on Diabetes Induced-Synaptic Fidelity in Brain Valencia Fernandes, Dharmendra Kumar Khatri, Shashi Bala Singh	144
34	Plasma Levels of Collagen Triple Helix Repeat Containing 1 (CTHRC1) as a Potential Biomarker in Interstitial Lung Disease Rijnbout-St.James Willem, Lindner Volkhard, Scholand Mary Beth, Ashton M. Tillett, Di Gennaro Michael Jude, Smith Silvia Enrica	145
35	Fraud Food and Food Spoilage Detection by Non-Destructive Technologies S. Khan, Z. Xiaobo	146
36	A Review of X-Ray for Detection of Insect Infestation in Fruits and Vegetables Suliman Khan	147
37	Chemical Analysis and Cytotoxic Evaluation of Asphodelus Aestivus Brot. Flowers Mai M. Farid, Mona El-Shabrawy, Sameh R. Hussein, Ahmed Elkhateeb, El-Said S. Abdel-Hameed, Mona M. Marzouk	148

38	Chemical Profiling of Farsetia Aegyptia Turra and Farsetia Longisiliqua Decne. and Their Chemosystematic Significance				
	Mona M. Marzouk, Ahmed Elkhateeb, Mona Elshabrawy, Mai M. Farid, Salwa A. Kawashty, EL-Sayed S. Abdel- Hameed, Sameh R. Hussein	149			
39	In Vitro and in Vivo Biological Investigations of Philodendron Bipinnatifidum Schott Ex Endl (Araceae) and Its Bioactive Phenolic Constituents Alia Ragheb	150			
40	Absence of Vancomycin-Resistant Enterococci Amongst Urban and Rural Hooded Crows in Hungary Isma Benmazouz, Bálint Joszef Nagy, Bence Bálacs, Gábor Kardos, László Kővér	151			
41	Cytotoxic Activity Of Major Iridoids From Barleria Trispinosa (Forssk.) Vahl. Growing In Saudi Arabia Hamza Assiry, Gamal A. Mohamed, Sabrin R. M. Ibrahim, Hossam M. Abdallah	152			

Parallel pipelined CG Algorithm on Heterogeneous Platforms

Sergey Kopysov, Nikita Nedozhogin, and Leonid Tonkov.

Abstract—The article presents a parallel iterative solver for large sparse linear systems which can be used on a heterogeneous platform. Traditionally, the problem of solving linear systems does not scale well on multi-CPU/multi-GPUs clusters. For example, most of the attempts to implement the classical conjugate gradient method were at best counted in the same amount of time as the problem was enlarged. The paper proposes the pipelined variant of the conjugate gradient method (PCG), a formulation that is potentially better suited for hybrid CPU/GPU computing since it requires only one synchronization point per one iteration, instead of two for standard CG. The standard and pipelined CG methods needs the vector entries generated by current GPU and other GPUs for matrix-vector product. So the communication between GPUs becomes a major performance bottleneck on miltiGPU cluster. The article presents an approach to minimize the communications between parallel parts of algorithms. Additionally, computation and communication can be overlapped to reduce the impact of data exchange. Using pipelined version of the CG method with one synchronization point, the possibility of asynchronous calculations and communications, load balancing between the CPU and GPU for solving the large linear systems allows for scalability. The algorithm is implemented with the combined use of technologies: MPI, OpenMP and CUDA. We show that almost optimum speed up on 8-CPU/2GPU may be reached (relatively to a one GPU execution). The parallelized solver achieves a speedup of up to 5.49 times on 16 NVIDIA Tesla GPUs, as compared to a one GPU.

Keywords—Conjugate Gradient, GPU, parallel programming, pipelined algorithm.

I. INTRODUCTION

IGHLY heterogeneous HPC platforms, where multicore processors are coupled with graphics processing units (GPUs), have been widely used in high performance computing as one approach to continuing performance improvement while managing the new challenge of energy efficiency [1]. Although some software packages and programming languages could be used directly, the introduction of multicore processors in HPC resulted in redesign of some critical software packages and significant refactoring of some existing parallel applications. Computing accelerators are contained in the computing nodes of supercomputers and are used quite successfully in solving many computing problems despite the fact that the central processor (CPU) is idle after running the core functions on the accelerator.

Each architecture of the CPU and GPU has unique features and, accordingly, is focused on solving certain tasks for which typical, for example, high performance or low latency. Hybrid

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CPU/GPU computing is one method of realizing performance gains independent of the iterative method used. With hybrid CPU/GPU computing, we focus on separating the computationally intensive portions of the program among several workers, taking into account their different productivity.

Currently, many parallel algorithms have been proposed that provide high performance and scalability when solving large sparse systems of equations on modern multiprocessor with a hierarchical architecture.

In [2] proposes a combination of a hybrid CPU-GPU and a pure GPU software implementation of a direct algorithm for solving shifted linear systems with a large number of complex shifts and multiple right-hand sides.

In [2] proposes one of the implementations of the software of a direct algorithm for solving shifting linear systems with a large number of complex shifts and multiple right-hand sides. This implementation combines hybrid CPU and GPU and a pure GPU software implementation. The construction of hybrid solvers with a combination of direct and iterative methods for solving SLAE allows the use of several levels of parallelism [3]–[7]. The separate steps of the CG algorithm are executed on a CPU or GPU, such as a preconditioner [8].

In [9] task scheduling on Multi-CPUs/Multi-GPUs platforms for the classical CG from the PARALUTION library is executed in the StarPU. It's unified runtime system for heterogeneous multicore architectures which is developed in the INRIA laboratory (France).

Our team considered one of the approaches a hybrid method for solving systems of equations of Schur complement by preconditioned iterative methods from Krylov subspaces was built and implemented when used together the cores of central (CPU) and graphic processing units (GPU) [10]. The classical preconditioned conjugate gradient method(PCG) [11] was applied for the block ordered matrix and the separation of calculations in matrix operations between the CPU and one or more GPUs, when the system of equations in Schur complement was solved in parallel.

The Krylov subspace methods are some of the most effective options for solving large-scale linear algebra problems. However, the classical Krylov subspace algorithms do not scale well on modern architectures due to the bottleneck related to synchronization of computations. Pipeline methods of the Krylov subspace [12] with hidden communications provide high parallel scalability due to the global communications overlapping with computing, performing matrix-vector and dot products. The first work on reducing communications was related to a variant of the conjugate gradient method, having one communication at each iteration [13], using the three-term

recurrence relations CG [14].

The next stage of development was the emergence of s-step methods from Krylov subspaces [15], in which the iterative process in the s-block uses various bases of Krylov subspaces. As a result, it was possible to reduce the number of synchronization points to one per s iterations. However, for a large number of processors (cores), communications can still take significantly longer than computing a single matrix-vector product. In [16] it was proposed a CG algorithm using auxiliary vectors and transferring a sequential dependence between the computing of matrix-vector product and scalar products of vectors. In this approach, the latency of communications is replaced by additional calculations.

In this paper, we consider the pipelined variant, which is potentially better for heterogeneous multi-CPUs/multi-GPUs computing, since it requires only one synchronization point per iteration, instead of two for standard CG.

This paper presents a pipeline technique for conjugate gradient method and discusses its parallel implementation on multi-CPU/multi-GPU platform for solving large sparse linear systems. Hybrid parallel computing approaches are adopted to significantly improve performance of the solver. Specifically, we introduce a hybrid solution by fully utilizing multi-core nodes available through multi-threading techniques by means of OpenMP, and exploit an access to massively parallel hardware through GPU-offloading with CUDA, in which data are transfered to the GPU for processing. The combination of GPU-offloading and CPU-threading is explored through a hybrid CPU/GPU compute implementation.

In our work, we modify the basic CG algorithm to minimize the cost of collective communication. A modified but mathematically equal variant of the conjugate gradient algorithm is employed to reduce the cost of global communication. By using the modified algorithm, the three vector dot products in each iteration can be done simultaneously with only one nonblocking collective communication that can be further overlapped with other operations.

II. PIPELINED ALGORITHM OF THE CONJUGATE GRADIENT $\begin{tabular}{ll} METHOD \end{tabular}$

We consider now the pipelined version of the conjugate gradient method, which is mathematically equivalent to the classical form of the preconditioned CG method and has the same convergence rate.

In this algorithm, the modification of the vectors r_{j+1} , x_{j+1} , s_{j+1} , p_{j+1} and matrix-vector products provides pipeline computations. The computation of dot products (line 4) can be overlapped with the computation of the product by the preconditioner (line 2) and the matrix-vector product (line 3). However, the number of triads in the algorithm increases to eight, in contrast to three for the classic version and four in [15]. In this case, a parallel computation of triads and two dot products at the beginning of the iterative process and one synchronization point is possible.

The pipelined version CG presented in this work can be used with any preconditioner. There are two ways to organize computations in the preconditioned pipelined CG, which provide a compromise between scalability and the total number

Algorithm 1 Pipelined algorithm CGwO.

```
1 r = b - Ax
u = M^{-1}r
3 \ w = Au
4 \gamma_1 = (r, u)
5 \delta = (w, u)
6 while ||r||_2/||b||_2 > \varepsilon do
       m = M^{-1}w;
      n=Am
9
       if (j=0) then
         \beta = 0
10
11
       else
12
          \beta = \gamma_1/\gamma_0
13
       end if
14
       \alpha = \gamma_1/(\delta - \beta \gamma_1/\alpha)
       z = n + \beta z; w = w - \alpha z; s = w + \beta s; r = r - \alpha s
15
       p = u + \beta p; x = x + \alpha p; q = m + \beta q; u = u + \alpha q
16
17
       \gamma_1 = (r, u); \ \delta = (w, u)
19 end while
```

of operations. Thus, the CG pipeline scheme is characterized by a different order of computations, the presence of global communication, which can overlap with local computations, such as matrix-vector product and operations with a preconditioner, and the possibility of organizing asynchronous communications.

The two variants of the conjugate gradient method were compared: the classical scheme and the pipelined one. Table I presents the results of numerical experiments where the execution time of a sequential version of the classical CG and the CGwO pipelined scheme (Algorithm 1) executed on the CPU and GPU are shown. Note that in the variants for the GPU, joint computation of all dot products of vectors in one kernel function was implemented, independently of each other. For this, when starting the CUDA kernel, the dimension of the Grid hierarchy of CUDA threads was set in two-dimensional form: 3 sets of blocks, each for performing computations on its own pair of vectors. This allowed us to reduce the number of exchanges between the CPU and GPU memory, combining all the resulting scalars in one communication.

Matrices from the SuiteSparse Matrix Collection [17] were used in the test computations. The right hand side vector was formed as a row-wise sum of matrix elements. Thus, the solution of the system Ax = b, dimension $N \times N$ (with the number of nonzero elements nnz) is a vector $x = (1, 1, ..., 1)^T$.

For systems of equations of small dimension, the solution time on the CPU according to the classical CG scheme is significantly less than the GPU execution time for the same number of iterations (see Table I). For large systems, the costs of synchronization and forwarding between the CPU and GPU overlap with the speed of the GPU. In the pipelined version of CGwO, the computational execution costs on the GPU are reduced almost threefold for all the considered systems of equations only due to the reduction of exchanges between the GPU and the CPU in the computation of dot products.

III. CG WITH THE COMBINED USE OF CPU AND GPU

Let us consider the application of the Algorithm 1 for the parallel solution of super-large systems of equations on computing nodes, each of which contains several CPUs and GPUs. To solve SLAEs on several GPUs, we construct a block pipelined algorithm for the conjugate gradient method. On heterogeneous platform, data exchange between different GPUs within the same computing node is carried out with OpenMP technology, and the exchange between different computing nodes is carried out by MPI technology.

For example, consider a node containing a central eightcore processor and two graphics accelerators. The number of OpenMP threads is selected by the number of available CPU cores. The first two OpenMP threads are responsible for exchanging data and running on two GPUs. Threads 2-6 provide computations on the CPU and can perform computations on a block of the SLAE matrix. The last thread provides data exchange with other computing nodes by MPI.

A. Matrix partitioning

To divide the matrix A into blocks, we construct the graph $G_A(V, E)$, where $V = \{i\}$ is the set of vertices associated with the row index of the matrix (the number of vertices is equal to the number of rows of the matrix A); $E = \{(i, j)\}$ is the set of edges. Two vertices i and j are considered to be connected if the matrix A has a nonzero element with indices i and j. The resulting graph is divided into subgraphs whose

For example, to split a graph, you can use the [18] layerby-layer partitioning algorithm, which reduces communication costs due to the need to exchange only with two neighboring computing nodes.

After that, each vertex of the graph is assigned its own GPU or CPU. On each computing unit, the vertices are divided into internal and boundary. The latter are connected with at least one vertex belonging to another subgraph.

After partitioning, each block A_k of the original matrix Acontains the following submatrices:

- $A_k^{[i_k,i_k]}$ matrix associated with the internal vertices; $A_k^{[i_k,b_k]}$, $A_k^{[b_k,i_k]}$ matrices associated with the internal and boundary vertices;
- $A_k^{[b_k,b_l]}$ matrix associated with the boundary vertices of the k-th and l-th blocks.

$$A = \begin{pmatrix} A_1^{[i_1,i_1]} & A_1^{[i_1,b_1]} & \cdots & 0 & 0 \\ A_1^{[b_1,i_1]} & A_1^{[b_1,b_1]} & \cdots & 0 & A_1^{[b_1,b_d]} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & A_d^{[i_d,i_d]} & A_d^{[i_d,b_d]} \\ 0 & A_d^{[b_d,b_1]} & \cdots & A_d^{[b_d,i_d]} & A_d^{[b_d,b_d]} \end{pmatrix}.$$

We divide the matrix-vector product n = Am into two components by using the obtained partition:

$$n_k^b = A_k^{[b_k,i_k]} m_k^i + \sum_{l=1}^{l \leq d} A_k^{[b_k,b_l]} m_l^b, \quad n_k^i = A_k^{[i_k,i_k]} m_k^i + A_k^{[i_k,b_k]} n_k^i$$

Here k corresponds to the computing device. The block representation of the vectors involved in the algorithm is inherited from the matrix partitioning. For example, the vector m has the form $m^T = (m_1^i, m_1^b, \dots, m_k^i, m_k^b, \dots, m_d^i, m_d^b)$. The implementation of the matrix-vector product reduces the cost of communication between blocks at each iteration of conjugate gradient method. To perform this operation, an exchange of vectors m_k^b is required, the size of which is less than the dimension of the initial vector m.

The partitioning of the preconditioner M is carried out in a similar way.

B. Block pipelined algorithm

The matrix blocks were mapped on the available CPU and GPU with the block partitioning of the matrix and vectors. The number and size of blocks let on to map the load in accordance with the performance of the computing units, including the allocation of several blocks to one.

Let us represent parallel block scheme of the method CGwO that is performed each k-th computing unit in the form of Algorithm 2. Two parallel branches of this algorithm are executed accordingly on the CPU and CPU/GPU. Operations performed in parallel are shown in one line of the algorithm. Vector operations on each computing unit occur in two stages, for internal and boundary nodes. The designations of the internal and boundary nodes for vectors are omitted, with the exception of the matrix-vector multiplication. Dot products are performed independently by each computing unit on its parts of vectors. The summation of intermediate scalars occurs in parallel threads responsible for communication, which is the synchronization point at each iteration of the algorithm.

In block CGwO, compared to Algorithm 1, the preconditioning step has been moved (line 7 to line 20). This is done in order to combine vector operations on the computing unit and the assembly of the vector parts of the right hand side to perform matrix-vector multiplication in preconditioning. The 31 line on the right uses the ternary operator: if j = 0, then $\beta = 0$, in other cases $\beta = \gamma_1/\gamma_0$. The subscript h is used for vectors that are stored only in CPU memory.

C. MPI+OpenMP+CUDA programming model

Numerical experiments on the Algorithm 2 were carried out on heterogeneous platform with various configuration of computing nodes containing several CPUs and GPUs. In the general case, the parallel computing on several heterogeneous computing nodes containing one or more CPUs and several GPUs is implemented by the combination of several technologies: MPI, OpenMP and CUDA. In this article, the approach is to properly divide the computational workload between the CPU and the GPU, so that the CPU can aid the GPU in sharing the computational costs. Our programming strategy is based on implementation strategy, where a hybrid MPI+CUDA+OpenMP programming model is used to realize concurrent CPU+GPU computations. The principal concept for $n_k^b = A_k^{[b_k,i_k]} m_k^i + \sum_{l=1}^{l \leq d} A_k^{[b_k,b_l]} m_l^b, \quad n_k^i = A_k^{[i_k,i_k]} m_k^i + A_k^{[i_k,b_k]} n_k^b \text{the strategy is to overlap computation with communication using OpenMPs nested parallelism capability to generate two$ independent groups of threads. The first thread group handles

Algorithm 2 Block algorithm CGwO performed on k-th device

```
Require: Matrix partitioning into blocks A_k^{[i_k,i_k]}, A_k^{[i_k,b_k]}, A_k^{[b_k,i_k]}, A_k^{[b_k,b_k]}.
   1 r = b
    u = M^{-1}r
         Parallel algorithm branches
    \begin{aligned} & (\mathbf{CPU} \vee \mathbf{GPU})_k \\ \mathbf{3} \ \ w_k^i &= A_k^{[i_k,i_k]} \cdot u_k^i + A_k^{[i_k,b_k]} \cdot u_k^b \\ \mathbf{4} \ \ w_k^b &= A_k^{[b_k,b_k]} \cdot u_k^b + A_k^{[b_k,i_k]} \cdot u_k^i \end{aligned} 
                                                                                                                     24 Assembly of the vectors u_k^b 25 w_h^b = \sum_{l=1,l\neq k}^{l\leq d} A_k^{[b_k,b_l]} \cdot u_k^b 26 Copying w_h^b on the GPU_k
   \begin{array}{ll} \mathbf{5} & w_k^b = w_k^b + w_h^b \\ \mathbf{6} & m = M^{-1}w \end{array}
                                                                                                                     27 Assembly of the vectors m_k^b 28 Assembly \delta=\sum_k \delta_k; \gamma_1=\sum_k \gamma_{1k}
   7 \gamma_{1k} = (r_k, u_k); \, \delta_k = (w_k, u_k)
  8 while ||r||_2/||b||_2 > \varepsilon do

9 n_k^i = A_k^{[i_k, i_k]} \cdot m_k^i + A_k^{[i_k, b_k]} \cdot m_k^b

10 n_k^b = A_k^{[b_k, b_k]} \cdot m_k^b + A_k^{[b_k, i_k]} \cdot m_k^i
                                                                                                                     29 n_h^b = \sum_{l=1,l \neq k}^{l \leq d} A_k^{[b_k,b_l]} \cdot m_k^b
30 Copying n_h^b on the GPU_k
            n_k^b = n_k^b + n_h^bz = n + \beta z
  11
                                                                                                                      31 \beta = ((j=0)?0: \gamma_1/\gamma_0)
  12
                                                                                                                     32 \alpha = \gamma_1/(\delta - \beta \gamma_1/\alpha)
            w = w - \alpha z
  13
             q = m + \beta q
  14
  15
             s = w + \beta s
                                                                                                                     33 Assembly of the vectors w_k^b
  16
             p = u + \beta p
             x = x + \alpha p
  17
             r = r - \alpha s
  18
                                                                                                                      34 Assembly vectors m_k^b
              u = u + \alpha q
  19
              m = M^{-1}w
  20
                                                                                                                      35 Assembly \delta = \sum_k \delta_k; \gamma_1 = \sum_k \gamma_{1k}
  21
              \gamma_{1k} = (r_k, u_k); \ \delta_k = (w_k, u_k)
  23 end while
```

the CUDA, MPI communication and computation of the halo boundary points on the CPU using OpenMP threads. The second thread group computes the interior points on the CPU.

Let us consider the software organization of computations using as example some cluster, which includes two computing nodes (8-CPU cores and 2-GPUs). Each computing node is associated with a parallel MPI process. In a parallel process, 9 parallel OpenMP threads are generated, which is one more than the available CPU cores. The eighth OpenMP thread is responsible for communications between different computing nodes (using MPI technology, vector assembly using the Allgatherv function, adding scalars Allreduce) and various GPUs. In the 2 Algorithm, the operations performed by this thread are presented to the right. Zero and first OpenMP threads are the host threads for one of the available GPU devices and are responsible for transfer data between the GPU/CPU (calls to asynchronous copying functions) and auxiliary computations. Each available GPU device (further considered as a computing unit) is associated with one of the parallel OpenMP threads, which is responsible for transferring data between the GPU and CPU (calls to asynchronous copy functions) and participates with the eighth treads in matrix-vector product on boundary vertices (lines 25, 29 right column). The remaining parallel threads (second to seventh) perform the calculations as a separate computing unit for their matrix block. The operations performed by computing units in

the 2 Algorithm are shown on the left.

The preconditioning in lines 2, 6 and 20 implies the use of block matrix-vector multiplication of the form (1) considered above.

IV. NUMERIC RESULTS

To evaluate the presented algorithm, two series of tests were carried out: on synthetically generated matrices from HPCG test [19] and matrices takes from the University of Florida Sparse Matrix Collection [20].

A. Benchmarking with HPCG Matrices

The High Performance Conjugate Gradient (HPCG) [19] is a benchmark program that solves a sparse linear system arising in solving a three-dimensional heat diffusion problem. HPCG intends to solve the linear system generated from the finite difference discretization of the Poisson equation: $-\bigtriangleup u=b$, with homogeneous Dirichlet boundary conditions applied along the boundary of a three-dimensional cubic domain $\Omega.$ Based on a semistructured mesh with equidistant mesh spaces in the $x,\ y$ and z directions, respectively, the discretization employed in HPCG leads to a second-order accurate 27-point stencil.

The resulting sparse linear system has the following properties: A — sparse matrix with 27 nonzero entries per row for

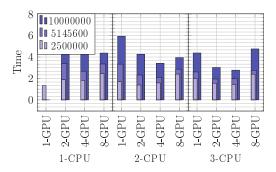


Fig. 1. Scalability of the block algorithms CGwO by CPU and GPU

interior equations and 7 to 18 nonzero terms for boundary equations; A — symmetric, positive definite, nonsingular linear operator.

We generate a synthetic symmetric positive definite (SPD) matrix A using an array-of-pointers-style compressed sparse row format, an exact solution vector of all 1.0 values, a corresponding right-hand-side vector b, and initial guess for x of all 0.0 values. The sparsity pattern of the synthetic matrix is really a regular 27-point 3-dimensional stencil pattern.

We tested one CPU performance on the Uran cluster based on three typical data sizes, including:

- 1) $125 \times 125 \times 160$, nnz = 66503662;
- 2) $160 \times 160 \times 201$, nnz = 137318884;
- 3) $200 \times 200 \times 250$, nnz = 267487792;
- 4) $250 \times 250 \times 310$, nnz = 519219712;
- 5) $310 \times 310 \times 390$, nnz = 1005862912;
- 6) $390 \times 390 \times 485$, nnz = 1986735009;

In all variants, the pipelined version of CG converged in 43 iterations with ε equal to 10^{-6} . For example, the solving time of the first three data sizes on one OpenMP thread were 8.39, 17.41, 33.22 seconds, respectively. We were able to obtain the result only for the first two sizes: 1.33, 2.72 when using single GPU. The remaining data sizes is not placed in the memory of one graphics accelerator. These results allow us to estimate that the performance of one OpenMP thread is approximately 6.5 times lower than the performance of single GPU for the linear system solving by the conjugate gradient method.

Performance metrices are executed and compared through scalability studies and absolute runtime results. To estimate the computational performance and the impact of MPI and OpenMP communications, our numerical experiments were executed with different numbers of CPUs and GPUs. The results are shown in the diagrams 1 and 2. Each diagram corresponds to the number of cluster nodes (n-CPU) involved in the computations and the number of graphics accelerators on each node (m-GPU).

The 3 diagram shows the results by subdomains for the case when 2 GPUs are used per computational node. Here, the matrix size of the linear system is approximately doubled. It can be noted that, starting from a size equal to 10,000,000, there is a good scalability of the algorithm. The problem execution time remains practically unchanged by doubling the problem size and doubling the number of subdomains.

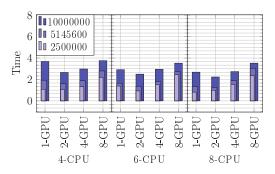


Fig. 2. Scalability of the block algorithms CGwO by CPU and GPU(continue)

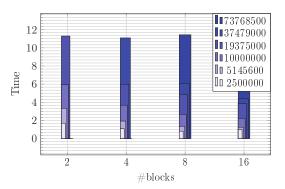


Fig. 3. Scalability of the block algorithms CGwO by number blocks

1

B. Benchmarking on the SuiteSparse Matrix Collection

The results of comparing two algorithms of the conjugate gradient method on SLAEs containing test matrices [19] are considered. The problems range from small matrices, used as counter-examples to hypotheses in sparse matrix research, to large test cases arising in large-scale computation.

In the standard PCG algorithm, three dot products need to be done per iteration, with each one requiring a global collective communication that may substantially degrade the scalability at scale. In order to reduce the global communication overhead, we employ a reformulated but mathematically equivalent variant of the basic PCG algorithm, the pipelined Block PCG.

As shown in Algorithm 2, the pipelined PCG method has two advantages. First, only one global reduction is required for each iteration. Second, the global reduction can be overlapped with the matrix-vector product and with the application of the preconditioner.

Figure 4 presents the results of accelerating the block algorithms of the conjugate gradient method, when divided

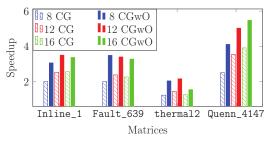


Fig. 4. Speedup of the block algorithms CG and CGwO

into a larger number of blocks, accordingly 8, 12 and 16. To compute the speedup, parallel application was run repeatedly with different mapping of subdomains to several CPUs and GPUs. For example, in the case of 12 subdomains, variants were considered: 2 CPUs with 6 GPUs, 3 CPUs with 4 GPUs, 6 CPUs with 2 GPUs. The best time is shown.

The results of comparing two algorithms of the conjugate gradient method on SLAEs containing test matrices are presented in Table I. The results are given for several types of computing nodes using a single graphics accelerator.

The matrices are ordered by increasing the order of the system of equations (N) and the number of nonzero elements (nnz). Bold indicates the best time to solve the system in each case. The pipelined algorithm CGwO showed a reduction in execution time on small SLAEs which are characterized by a small computing load, due to which a reduction in communications provides less time. Note that the classic CG algorithm was implemented based on CUBLAS, while the CGwO variant uses matrix and vector operations of its own GPU implementation.

For systems Inline_1 and Fault_639, the execution time of the pipelined algorithm is 10 and 13.5% longer than the block version of CG, which is associated with additional vector operations that are not blocked by reduced communications. With a decrease in the number of iterations, for example, for solving a large system with G3_circuit) with an approximately equal number of equations with thermal2, the execution time of the CG and CGwO algorithms on one GPU increases slightly. For the system (thermal2 and G3_circuit) the increase in costs becomes more significant.

Table II presents the results of the block variant of the algorithms for computing on several computing nodes for systems with small dimension matrices. Here are the results for 2 and 3 subdomains. Each subdomain was considered on a separate computing node. Communications were carried out using MPI technology. A significant influence of network characteristics on the performance of block methods can be seen in Table II for system of equations with matrix 1138_bus. Computations for these SLAEs were performed at various computing nodes with different throughput and latency of the network. In numerical experiments on the CNs (partition "debug") connected by a Gigabit network, communication costs significantly increase the execution time of the CG algorithm. For example, in the variant 1138_bus on the cluster partition "debug", the execution time of the pipeline algorithm is 3.6 times less (the line "debug" in Table II and any row in Table I). Using the Infiniband 20 Gb/s communication network reduces the execution time for all presented systems of equations (lines "M2090" and "K40m").

When reducing the computational load, a decrease in the number of synchronization points and the consolidation of transfers per transaction is more pronounced. This shows a comparison of systems with matrices Kuu and Muu. Both systems have an equal number of equations and nonzero elements, but the conditionality of these matrices is significantly different and, as a consequence, the number of iterations in the conjugate gradient method is different. Table I shows that using the pipeline algorithm for the matrix Muu gives

speedup by 70 times, compared with the matrix Kuu, where the speedup is only 2.8.

The speedup was considered relative to the option on one GPU from Table I. An application that implements this algorithm was executed in the exclusive mode of the computing node but not of the network.

As can be seen from the presented results, the pipelined CG shows the speedup greater than the classic version of conjugate gradient method. Wherein, for the largest of the considered matrices Quenn_4147, the speedup achieves 5.49 times, while the classical version gives 3.92 as maximum. For the strongly sparse matrix thermal2, block algorithms don't give high speedup (maximum is 1.56), since the computational load depends mainly on the number of the nonzero elements.

An analysis of the results showed that reducing the data size due to the matrix partitioning and reducing the synchronization points slightly decrease the impact of communication costs on the total algorithm performance. Only the use of computing nodes connected by Infiniband allowed us to get speedup when computing on several computing nodes. The matrix partitioning into blocks allowed to decrease the execution time of the pipelined block algorithm in comparison with the conjugate gradients on one node on the matrices Inline_1, Fault_639 by reducing the computational load on one GPU.

Large systems thermal2, G3_circuit, solved by the block of the CGwO algorithm, as well as the reduction in communications costs and synchronization points, do not overlap the increasing costs of additional vector operations.

V. CONCLUSION

The heterogeneous computing platforms containing and sharing CPU + GPUs provide an effective solution to a wider range of problems with high energy efficiency when CPU and GPUs are uniformly loaded.

The parallel implementation of the solution of systems of linear algebraic equations on a heterogeneous platform was considered. The performance of parallel algorithms for classical conjugate gradient method is significantly limited by synchronization points when using the CPU and GPU together. A pipelined algorithm of the conjugate gradient method with one synchronization point was proposed. Also, it is provided the possibility of asynchronous computations, load balancing between several GPUs located both on the same computing node and for a GPU cluster when solving systems of large-dimensional equations. To further increase the efficiency of calculations, it is supposed to study not only the communication load of the algorithms but also the distributing of the computational load between the CPU and GPU. To obtain more reliable evaluation of communications costs, it is necessary to conduct a series of computational experiments on supercomputer with a completely exclusive mode of operation and a large number of heterogeneous nodes.

The following conclusions can be drawn from the analysis of data obtained during numerical experiments: the use of a pipeline algorithm reduces communication costs, but increases computational ones. For systems of small sizes or with a small number of iterations, this reduces the execution time of the

TABLE I STATISTICS OF THE TEST PROBLEMS. PROBLEM NAMES, DIMENSIONS (N), NUMBER OF NONZEROS (nnz), DEVICE TYPE (DT) AND PROBLEM ANALYSIS IN TERMS OF THE TIMING IN SECONDS.

Matrix	N	nnz	# iter.	DT	Time, s	
					CG	CGwO
Plat362	362	5786	991	M2090	6.88E-01	3.07E-01
				K40m	4.13E-01	3.12E-01
1138_bus	1138	4054	717	M2090	3.81E-01	1.84E-01
				K40m	5.31E-01	2.01E-01
				debug	6.82E-01	1.90E-01
Muu	7102	170134	12	M2090	2.64E-01	4.68E-03
				K40m	3.31E-01	4.55E-03
Kuu	7102	340200	378	M2090	4.31E-01	1.31E-01
				K40m	4.39E-01	1.35E-01
Pres_Poisson	14822	715804	661	M2090	6.72E-01	3.13E-01
				K40m	6.346E-01	2.73E-01
Inline_1	503712	36816342	5642	M2090	4.74E+01	5.17E+01
				K40m	3.06E+01	3.37E+01
Fault_639	638802	28614564	4444	M2090	3.83E+01	4.32E+01
				K40m	2.44E+01	2.77E+01
				debug	2.44E+01	2.77E+01
thermal2	1228045	8580313	2493	M2090	1.35E+01	1.82E+01
				K40m	8.33E+00	1.18E+01
G3_circuit	1585478	7660826	592	M2090	3.43E+00	4.32E+00
				K40m	1.94E+00	2.92E+00
Quenn_4147	4147110	399499284	8257	M2090	5.46E+02	5.78E+02
				K40m	3.55E+02	3.75E+02

 $\label{thm:table II} Time of solving by the block algorithms CG and CGwO on CPU/GPU, s.$

Matrix/DT	CG/#	blocks	CGwO/#blocks	
Maura/Dr	2	3	2	3
Plat362/ M2090	1.55E+00		1.22E+00	
/K40m	1.92E+00	1.56E+00	1.28E+00	1.31E+00
1138_bus/ M2090	1.84E+00		9.28E-01	
/K40m	1.90E+00	1.85E+00	1.03E+00	1.04E+00
/debug	1.25E+01		5.36E+00	
Muu/ M 2090	6.12E-01		2.29E-01	
/K40m	6.59E-01	5.64E-01	2.89E-01	2.88E-01
Kuu /M2090	1.30E+00		6.43E-01	
/K40m	1.29E+00	1.36E+00	6.81E-01	7.95E-01
Pres_Poisson/M2090	1.55E+00		9.57E-01	
/K40m	1.60E+00	1.66E+00	1.02E+00	1.19E+00
G3_circuit/M2090	4.27E+00		3.99E+00	
/K40m	4.04E+00	3.510E+00	3.27E+00	2.77E+00

algorithm when using a single GPU. For systems of large dimensions, a reduction in execution time, in comparison with CG, is possible only with a sufficiently small partition of the matrix into blocks, in which the increased computing costs overlap the communication decrease.

The proposed block algorithms, in addition to reducing the execution time, allow solving large linear systems that requires memory resources not provided by one GPU or computing node. At the same time, the pipelined block algorithm reduces the overall execution time by reducing synchronization points and combining communications into one message.

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