AUGUST 3-8, 2015

2015 AARMS WORKSHOP
on DOMAIN DECOMPOSITION METHODS FOR PDEs

PROGRAM

AARMS (Atlantic Association for Research in the Mathematical Sciences), the AARMS Collaborative Research Group in Numerical Analysis and Scientific Computing at **Memorial University of Newfoundland**, and the Department of Mathematics and Statistics at **Dalhousie University** will bring researchers interested in parallel methods for partial differential equations to a 5-day workshop in beautiful Halifax, NS, Canada.

The meeting will consist of a 2-day short course on domain decomposition methods for PDEs taught by leading expert **Dr. Martin Gander** (University of Geneva), research level talks by experts in the area of domain decomposition and parallel methods, and talks by academic and industrial researchers with applied problems who have an interest in exploring parallel techniques. The final part of the workshop will be interactive, linking the applied researchers with domain decomposition experts to investigate the process of introducing parallelism into their simulations.

VENUE

Life Sciences Center/Chase Building/Dunn Building, **Dalhousie University**

PLENARY SPEAKERS

Victorita Dolean

University of Strathclyde

Martin Gander

University of Geneva

David Keyes

KAUST

Felix Kwok

Hong Kong Baptist University

ORGANIZERS

Hermann Brunner, Ronald Haynes, Scott MacLachlan

Memorial University

Paul Muir

Saint Mary's University

David Iron

Dalhousie University

APPLIED PROBLEM PRESENTERS

Tom Jönsthövel

Schlumberger

Hansong Tang

City University of New York

Rick Link, Neil McCormick

Lloyd's Register ATG/Martec

NSERC CRSNG

Ontario

THE FIELDS INSTITUTE FOR RESEARCH IN MATHEMATICAL SCIENCES

2015 AARMS Workshop on Domain Decomposition Methods for PDEs

Dear Workshop Participants,

We welcome you to the 2015 AARMS/CRM/Fields Workshop on Domain Decomposition Methods for PDEs, to be held Aug. 3rd-8th at Dalhousie University, Halifax, Nova Scotia, Canada. This workshop is the second in a series of workshops sponsored by the AARMS Collaborative Research Group in Numerical Analysis and Scientific Computing.

This year's workshop has four related components: a short course on domain decomposition methods for PDEs taught by Martin Gander (University of Geneva) with an associated hands-on software session by Victorita Dolean (University of Strathclyde), plenary research talks on the latest advances in domain decomposition methods by Martin Gander, Victorita Dolean, David Keyes (King Abdullah University of Science and Technology) and Felix Kwok (Hong Kong Baptist University), and applied problem presentations by Tom Jönsthövel (Schlumberger), Rick Link/Neil McCormick (Lloyd's Register ATG/Martec), and Hansong Tang (City University of New York), and interactive break-out sessions.

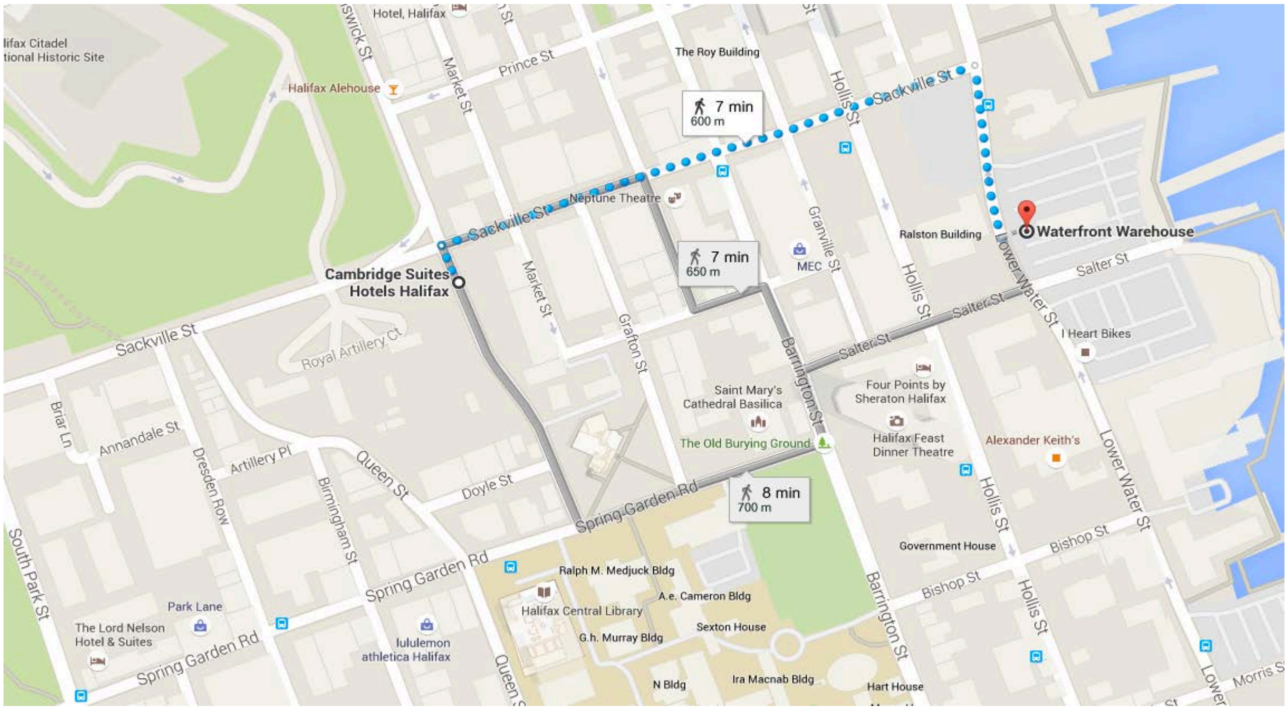
Our sincere thanks to our financial sponsors; these include the Fields Institute for Research in the Mathematical Sciences, the Atlantic Association for Research in the Mathematical Sciences, the Centre de Recherches Mathématiques, NSERC, Springboard Atlantic, the National Science Foundation in the United States, and Memorial University of Newfoundland.

This program contains the schedule for the workshop, as well as organizational information and a list of titles/abstracts for the speakers at the workshop.

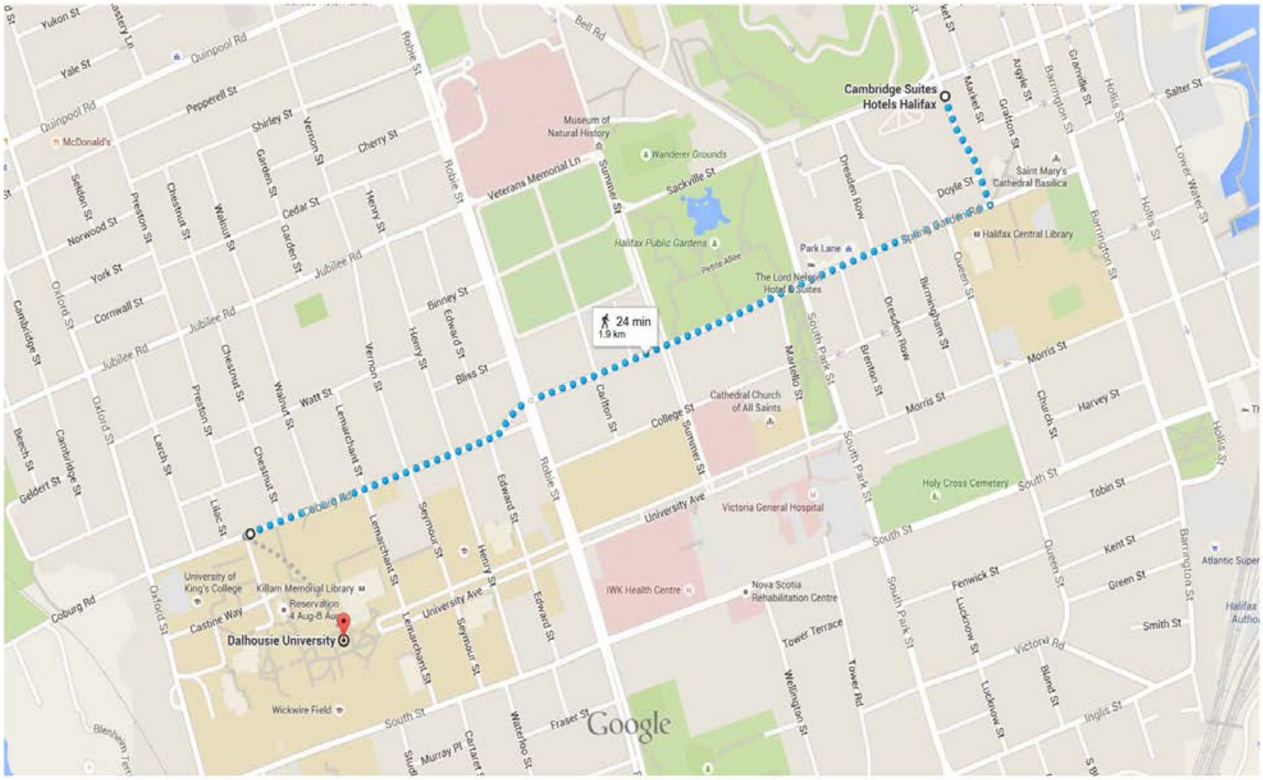
We wish you an interesting and productive time at the workshop and during your stay in Halifax!

Sincerely,
Hermann Brunner, Ronald Haynes, David Iron, Scott MacLachlan, and Paul Muir (Co-organizers)

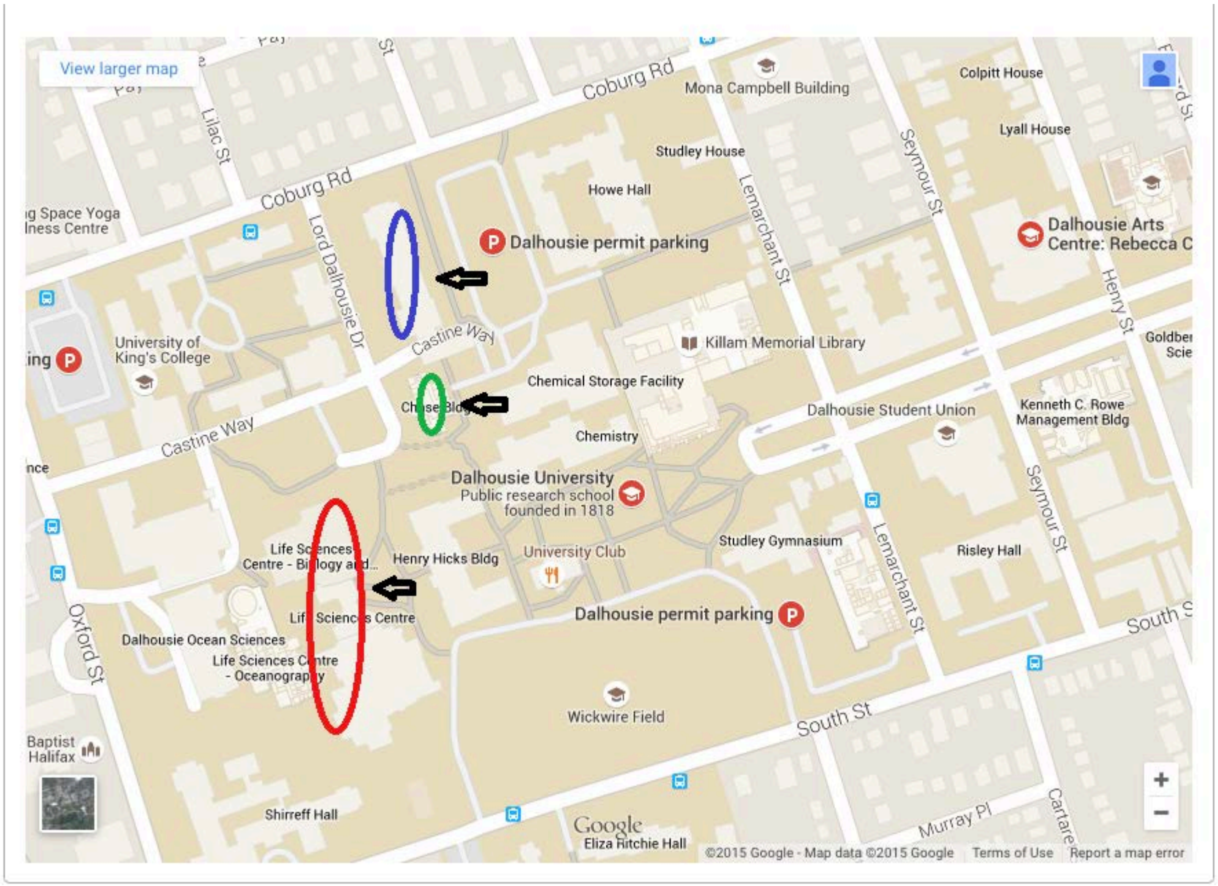
Cambridge Suites Hotel to Tug's Pub at the Waterfront Warehouse (Pub Night)



Cambridge Suites Hotel to Dalhousie University



Map of the Dalhousie Campus



- Life Sciences Center **(Red)**, Chase Building **(Green)**, Dunn Building **(Blue)**
- **To get to the main workshop room, enter the Chase Building** at the doors indicated by the black arrow. Go down the stairs, turn left, and then go left down the hall. Go through two doors and the main workshop room LSC206 is just outside the second door.

Food

- On campus: Student Union, Killiam Library, University Club, Howe Hall (see above map)
- Off campus: Walk out to Coburg Rd., turn right and walk to the traffic lights at Robie St.; there are many food establishments near this intersection.

WiFi

Eduroam (**edu**cation **roam**ing) is the secure, world-wide roaming access service developed for the international research and education community. Eduroam is available on campus as Dalhousie University is an Eduroam affiliated institution. Alternatively, please find enclosed in your workshop folder information on how to login using a guest account through the Dalhousie University wireless network.

Travel Reimbursement

For workshop participants who have been authorized to receive a travel reimbursement, the instructions for completing the reimbursement process are given below. **Note that the process for U.S. participants is different from the process for non-U.S. participants.** **Please save all original receipts associated with your travel claim.**

Non-U.S. Participants

Please download a Saint Mary's University Travel Expense form from
http://www.smu.ca/about/financial-services-forms.html#ExpenseReport

The form is available in either MS-Excel or pdf formats.
Additional information that may be of help in filling in the form is given at
http://www.smu.ca/about/financial-services-travel-and-insurance.html

Please fill in and sign the form and attach to the form all appropriate receipts such as airfare receipts, boarding passes, registration receipts, etc. . Please send your materials to:

AARMS Domain Decomposition Workshop,
c/o Rose Daurie,
Department of Mathematics and Computing Science,
Saint Mary's University,
Halifax, NS, Canada, B3H 3C3

Make sure to include your e-mail address with the materials you send in the event we need to follow up with you. **Note that you will only be reimbursed up to the amount that you have been authorized to claim in advance.**

U.S. Participants

Please submit your travel request using the cover page form available at
http://www.math.mun.ca/anasc/TravelNSF.pdf

Please fill in and sign this form and then **scan the form together with copies of all your receipts**, e.g., airfare receipts, boarding passes, registration receipts, etc., **all as ONE PDF file.**

Once the PDF file has been prepared, please e-mail the file to Gurpreet Kaur at gkaur@ccny.cuny.edu. Her office phone number 212-650-7900.

Please retain all original receipts until you receive the reimbursement check in case it is necessary to verify your expense claim. Failure to keep original receipts could result in a disallowance of the reimbursement for that expense. **Note that you will only be reimbursed up to the amount that you have been authorized to claim in advance.**

Schedule

>>> Monday, August 3, 2015, 6-8pm, OPENING RECEPTION, Cambridge Suites Hotel <<<

	Tues., Aug 4	Wed., Aug	Thurs., Aug 6	Fri., Aug 7	Sat., Aug 8
9:00-9:15 am	Coffee/ Welcome LSC-206	Coffee	Coffee	Coffee	Coffee
9:15-10:00 am	Short Course LSC-206	Short Course LSC-206	Applied 1 LSC-206 Tom Jönsthövel	Plenary 3 LSC-206 Victorita Dolean	Contributed 1/2 LSC-206 Christian Glusa Jianming Zhang
10:00-10:15 am	Break	Break	Break	Break	
10:15-11:00 am	Short Course LSC-206	Short Course LSC-206	Applied 2/3 LSC-206 Hansong Tang Rick Link/ Neil McCormick	Breakout #2 LSC-206 Chase-319 Chase-227	Break
11:00-11:15 am					Report on Breakout and Final Remarks LSC-206
11:15-12:00 noon	Software Prep Dunn-301A	Software Demo Dunn-301A			
12:00-2:00 pm	LUNCH	LUNCH	LUNCH	LUNCH	
2:00-2:15 pm			Intro to Breakout LSC-206		
2:15-3:00 pm	Short Course LSC-206	Short Course LSC-206	Breakout #1 LSC-206 Chase-319 Chase-227	Plenary 4 LSC-206 Martin Gander	
3:00-3:15 pm	Break	Break	Break	Break	
3:15-4:00 pm	Short Course LSC-206	Short Course LSC-206	Plenary 1/2 LSC-206 David Keyes Felix Kwok	Breakout # 3 LSC-206 Chase-319 Chase-227	
4:00-5:00 pm	Software Demo Dunn-301A	Software Demo Dunn-301A			
5:30-8:30 pm			Pub Night		

Plenary Talk Abstracts

David Keyes (King Abdullah University of Science and Technology)

Scalable Nonlinearly Implicit Methods for Multiscale Science and Engineering Applications

Many simulations must be followed over time intervals that are long compared to the shortest timescales in the system, e.g., convective versus acoustic timescales in aerodynamics, ocean turnover versus gravity wave timescales in climate, plasma discharge versus Alfven timescales in tokamaks, piston travel versus fast reaction timescales in internal combustion. Often, the phenomena associated with the shortest timescales may be assumed to be in equilibrium relative to dynamics of interest; however, they control the computational timestep if an explicit method is used, with the result that even weak scaling cannot be achieved. Often, as well, one would ideally employ a high-order timestepping scheme and take relatively large timesteps for computational economy; however, if operator splitting techniques are used the lower order splitting error thwarts this objective. For these and other reasons, fully implicit methods are increasingly important for the nonlinear multiscale applications that pace large-scale simulations in energy, environment, and other complex systems. The good news is that advances in domain decomposition methods for distributed memory parallel computers, globalization algorithms, and software that implements them without demanding that the user constructs a full Jacobian make implicit methods practical alternatives. Moreover, we argue that computational challenges on the immediate horizon - uncertainty quantification, inverse problems, multiphysics coupling, etc. - are most naturally tackled with fully nonlinearly implicit formulations for the underlying forward problems well in hand. We illustrate these claims for systems governed by partial differential equations.

Victorita Dolean (University of Strathclyde)

Robust Coarse Spaces via Generalised Eigenproblems: the GenEO method

The main motivation to build a roust coarse space for a two-level additive Schwarz method is to achieve scalability when solving highly heterogeneous problems i.e. for which the convergence properties do not depend on the variation of the coefficient. Recently, for scalar elliptic problems, operator dependent coarse spaces have been built in the case where coefficients are not resolved by the subdomain partition. A very useful tool for building coarse spaces for which the corresponding two-level method is robust, regardless of the partition into subdomains and of the coefficient distribution, is the solution of local generalised eigenvalue problems. In this spirit, for the Darcy problem, we proposed to solve local generalised eigenvalue problems on overlapping coarse patches and local contributions are then "glued together" via a partition of unity to obtain a global coarse space. We proposed a coarse space construction based on Generalized Eigenproblems in the Overlap (which we will refer to as the GenEO coarse space). This particular construction has been applied successfully to positive definite systems of PDEs discretized by finite elements with only a few extra assumptions.

Felix Kwok (Hong Kong Baptist University)

Schwarz Methods for the Time-Parallel Solution of Parabolic Control Problems

In optimal control problems, the goal is to find, for a given mechanical or biological system, the forcing function with minimal cost that drives the system to a desired target state. The numerical solution of optimal control problems under PDE constraints has become an active area of research in the past decade, with a growing list of applications such as the control of fluid flow governed by the Navier-Stokes equations, quantum control and medical applications related to the optimization of radiotherapy administration. When the governing PDE is parabolic, one must solve a coupled system of two PDEs, one forward in time (the state PDE) and another backward in time (the adjoint PDE). The tight coupling between these equations leads to extreme computational and storage requirements, so parallelization is essential. A natural idea is to apply Schwarz preconditioners to the large space-time discretized problem. Because the problem is essentially a two-point boundary value problem in time, it is possible to parallelize in time just as effectively as in space. We present a convergence analysis for a class of Schwarz methods applied to a decomposition of the time horizon into many subintervals. We show that just applying a classical Schwarz method in time already implies better transmission conditions than the ones usually used in the elliptic case, and we propose an even better variant based on optimized Schwarz theory.

Martin Gander (University of Geneva)

Five Decades of Time Parallel Time Integration

Time parallel time integration methods have received renewed interest over the last decade because of the advent of massively parallel computers, which is mainly due to the clock speed limit reached on today's processors. When solving time dependent partial differential equations, the time direction is usually not used for parallelization. But when parallelization in space saturates, the time direction offers itself as a further direction for parallelization. The time direction is however special, and for evolution problems there is a causality principle: the solution later in time is affected (it is even determined) by the solution earlier in time, but not the other way round. Algorithms trying to use the time direction for parallelization must therefore be special, and take this very different property of the time dimension into account. I will show in this talk how time domain decomposition methods were invented, and give an overview of the existing techniques. Time parallel methods can be classified into four different groups: methods based on multiple shooting, methods based on domain decomposition and waveform relaxation, space-time multigrid methods and direct time parallel methods. I will show for each of these techniques the main inventions over time by choosing specific publications and explaining the core ideas of the authors. This talk is for people who want to quickly gain an overview of the exciting and rapidly developing area of research on time parallel methods.

Software Demo Abstract

Victorita Dolean (University of Strathclyde)

The purpose of this presentation is to offer an overview of the most popular domain decomposition methods for partial differential equations (PDE). The presentation is kept as much as possible at an elementary level with a special focus on the definitions of these methods in terms both of PDEs and of the sparse matrices arising from their discretizations. We also provide implementations written in an open source finite element software FreeFem++ linked to the MPI-C++ framework HPDDM. In addition, we consider a number of methods that are not present in other libraries.

Reference: V. Dolean, P. Jolivet and F. Nataf, Introduction to Domain Decomposition Methods: algorithms, theory and parallel implementation", 2015.

Applied Problem Talk Abstracts

Tom Jönsthövel (Schlumberger)

In reservoir simulation we predict the recovery of gas and oil by solving for the fluid flow in porous media. Our reservoir simulator is designed from the ground up to run in parallel to speed up the computations and to reduce the overall simulation time. In general we distinguish between two properties when assessing the performance of an algorithm executed in parallel: weak and strong scalability. Weak scalability is the “speed up” which results from increasing the number of processors and keeping the same problem size per processor. In the ideal case we want to solve twice the problem size in the same time given twice the number of processors.

Strong scalability is defined as the speed up which results from increasing the number of processors and freezing the original problem size. In the ideal case we solve the original problem in half the time given twice the number of processors. In reality these ideal scenarios are hard to achieve because of latency in communication, i.e. there exists no communication between processors with infinite speed. Moreover, we pay a penalty when the ratio between communication and the actual amount of work per processor becomes unfavorable. This means that a processor is without work while waiting for data from neighboring processors.

The time-dependent, non-linear equations which underlie reservoir simulation are discretized by the Finite Volume method and solved by the Newton-Raphson method and implicit time integration. In every step of the Newton-Raphson method we evaluate the derivatives of the non-linear reservoir simulation equations and solve the corresponding linear system. Typically for a simulation of cells we solve for unknowns, with unknowns per cell. These are pressure, water (and gas) saturations and molefractions.

The matrices in the resulting linear systems are non-symmetric. We solve these systems with FGMRES preconditioned by the constrained pressure residual (CPR). To tackle the two different numerical properties of the discrete operator, elliptic and hyperbolic, we have two stages in CPR: 1st stage solve the pressure equations, 2nd stage solve the complete system. We solve the 1st stage by AMG and the 2nd stage by block-ILU(k), where k is 0 or 1.

The AMG solver is the bottleneck of this algorithm. It takes considerable amount of time, mostly in the setup. AMG is the state-of-the-art and (near-) optimal for solving elliptic equations. Moreover, AMG is well known for its excellent weak scalability property, it scales well for increasingly bigger problem sizes. However, the strong scalability of AMG is poor. The poor strong scalability of AMG is a critical business issue as clients expect to run cases (considerably) faster when running cases of fixed size on a cluster.

The aim of this workshop is to explore if domain decomposition methods can improve the strong scalability of the pressure solver.

Hansong Tang (City University of New York)

Methods and Applications of Domain Decomposition for Fluid Flows

Objective This talk presents fundamentals as well as current status of DD for fluid flows, and its applications in fronts of various computational physics and engineering problems. The materials include classic work in DD for fluids as well as the author's work in this area in many years.

Content

I. Domain decomposition for hyperbolic conservation laws

As a theoretical foundation of governing equations for fluid flows, hyperbolic conservation laws and their discretization will be introduced. On this basis, DD methods to compute the conservation laws will be presented and analyzed with regard to their consistency, stability, and convergence. Typical algorithms at grid interfaces are presented, and one and higher dimensional situations will be discussed. Ref., e.g., [1--7]. The topics are

- An overview
- Interface algorithms
- Conservation error, stability, and weak solutions

II. DD for compressible flows

DD methods for compressible flows with backgrounds in aerospace engineering will be discussed, with emphasis on algorithms for treatments at grid interfaces. Difficulties including accurately and correctly capturing shock at grid interfaces will be illustrated and methods to overcome them will be presented. Ref., e.g., [4, 7-11]. The topics are

- Conservative and non-conservative Interface algorithms
- Interface treatments and non-physical solution

III. DD for incompressible flows

Methods for computing 3D, unsteady, incompressible flows are discussed, and several typical algorithms will be introduced, including a simple, effective algorithm proposed by the author for overset grids. Ref. [12--17]. The topics are

- Mass flux based-interpolation for grid interface
- Application to flows with complex geometry

IV. DD for environmental flows

Simulation of several important yet difficult environmental flow problems in actual engineering projects will be presented to illustrate the necessities and advantages of DD, which include stratified flows in reservoir and near fish intake, initial mixing of thermal effluent flows, etc. Ref. e.g., [14, 18].

V. DD for multiscale and multiphysics coastal ocean flows

Numerical simulation of coastal ocean flows has been greatly successful, but, strictly speaking, it is restricted to large-scale flows and individual phenomena. In recent years, various multiscale, multiphysics coastal ocean flows are emerging, such as Mexico Gulf oil spill and storm surge impinging and damaging bridges, and it has become urgent to develop our capability to simulate such flows. In view that there exist many mature models for individual phenomena at specific scales, coupling of these models via DD is the most promising and feasible approach for us to achieve such capability. In this talk, we will present our effort on integration of SIFOM, a model for smallscale, fully 3D, incompressible flows, and FVCOM, a model for estuary-scale coastal ocean flows via DD implemented with an overset grid method. The DD is not trivial; it involves coupling of different sets of PEDs, distinct algorithms, and dissimilar grids. Such effort is the first of its kind, and can deal with many mutliphysics phenomena spanning a vast range of scales that are beyond the reach of other existing models. Numerical experiments on solution accuracy, convergence, etc. of the SIFOM-FVOCM system and its applications will be presented. Ref., e.g., [19—21].

VI. Challenges and open questions

A crucial issue in DD for fluids is grid interface treatment, and it has been studied intensively for incompressible flows in 1980s and 90s with regard to accuracy, stability, and convergence [5-11]. Now we are making efforts in integration of different flow models for coastal ocean flows (incompressible, with free surfaces) via DD [19-21], which involves coupling of different sets of PEDs, distinct algorithms, and dissimilar grids and is at fronts of DD and far more complicated than past DD problems. We will present involved open questions with regard to

- Model connection conditions leading to well posedness of the problems
- Model interface schemes that strictly assure certain properties such as conservation of mass

Progress on above issues will set up correct and solid foundations of above effort and produce seamless transition of solutions between different models and physical solutions.

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Rick Link and Neil McCormick (Lloyd's Register ATG/Martec)

Potential Applications For Domain Decomposition Methods At Lloyd's Register ATG

For 40+ years, Lloyd's Register (LR) ATG has been performing numerical simulations of engineering problems, including structural, fluid, thermal, and acoustical applications. Our Chinook computational fluid dynamics (CFD) software solves large compressible flow problems, such as explosive and supersonic turbulent flow problems, using domain decomposition (DD) methods to solve the 3-D Euler and Navier-Stokes equations. Problems are run using Beowulf clusters with MPI, and Metis for computing load-balanced partitions.

For problems involving adaptive mesh refinement (AMR) or discrete particle analysis, it is difficult to maintain grid load balancing, due to the changing problem topology. It is of interest to investigate strategies which minimize repartitioning time. It is also desired to determine whether there have been significant advances in other DD technology from Chinook's current status.

LR ATG performs finite element (FE) analyses of large ship problems using our flagship structural solver, VAST, which involves the inversion of a large, sparse matrix system. To reduce the number of degrees of freedom, ship models are usually composed of degenerate geometry in the form of shell and beam elements. These elements have high ratios of membrane to bending stiffness, which cause convergence difficulties for iterative solvers. No preconditioners have been found which adequately deal with all problems, hence the continued use of direct solvers in commercial FE packages.

There have been many advances in direct solvers in the last 20 years, including the invention of the supernodal method, which allows fast computation of dense matrix structures. The current linear solver in VAST utilizes Intel's Math Kernal Library (MKL) to perform this dense arithmetic. However, new methods utilize Schur decomposition, in which the structural mesh is broken into partitions that are initially solved independently. The second phase then involves the solution of the mesh region connecting the partitions. These methods are of interest to LR ATG, since they are applicable to both shared and distributed computing environments, and are almost directly scalable.

Contributed Talk Abstracts

Jianming Zhang (Hunan University)

Multi-domain Boundary Face Method for Thermal Analysis of Gravity Dams and its Possible Implementation by Domain Decomposition Methods

Within a successful CAE driven product development, there are two fundamental issues: a seamless interaction between the CAD and CAE software tools and a fast solver for large scale computation. This paper applies the boundary face method (BFM) to solve the steady-state and transient heat conduction problems occurs in gravity dams construction. Compared with the traditional BEM, the BFM performs the boundary integration on the boundary faces, which are represented in parametric form exactly as the boundary representation (Brep) data structure in solid modeling. Therefore, the BFM has potential to make direct use of a body's parametric representation, which is available in most of CAD packages, and thus, to be seamlessly integrated into CAD environments.

Meanwhile, discretization of a gravity dam may result in a large number of elements, up to millions usually, making the computational scale extremely large. The non-local kernels of the integral operator in the BIE makes the situation even worse. As the coefficient matrix is fully populated, both the memory requirement and CPU time for solving the system equation are of O(N2) complexity, where N is the number of unknowns. Among the so far available accelerating methods that can dramatically reduce the memory and computational time, the Hierarchical Matrix combined with ACA is a purely algebraic algorithm, and can be easily integrated into existing BEM codes. In this work, we adopt the ACA to accelerate the BFM computation.

Our contributions are as follows:
1) Integrated the BFM into UG-NX, making the CAE entirely within the CAD environment.
2) Implemented quasi-initial condition method for transient thermal problems, and proposed a time step scaling method to solve the instability problem occurs in case of small time step. (The time steps in dam simulation are relatively small, as the heat conductivity of concrete is small but its hydration speed is large)
3) Proposed a geometric mapping cross approximation (GMCA) method, which is equivalent to ACA but without iteration. The GMCA makes the low-rank representation of the BIE more convenient and efficient.
4) Proposed two kinds of new elements, i.e. pipe element and element with negative parts. These elements has been successfully used to deal with cooling water pipes in dam.
5) Proposed a domain sequence optimization method for multi-domain problems, which can deal with arbitrary inter-domain connections and get best efficiency by optimizing the band of the assembling system matrix.

Application examples of dam construction simulation are presented and the possible combination with Domain Decomposition Method to account for multi-domain problems is discussed using real engineering examples.

Christian Glusa (Brown University)

Multigrid Methods, Random Matrices and Fault Resilience

Exascale computing is expected to be obtained within the next several years. As error rates per component are unlikely to improve, high performance computing will have to handle different fault scenarios. In this talk, we analyze the behavior of two- and multigrid methods under the action of random node failures. Employing tools from random matrix theory, we develop a fault-resilient algorithm, give analytic convergence estimates, and show simulation results.
(Joint work with Mark Ainsworth)