The Local Organizing Committee

Ronald D. Haynes
Scott MacLachlan
Hermann Brunner
Sue Brenner
Shaun Lui
Emmanuel Lorin

Sponsors:

We also recognize the support of the Faculty of Engineering at Memorial, Department of Mathematics and Statistics, Lawrence Livermore National Laboratory and Los Alamos National Laboratory in the United States.
International Scientific Committee

Bjørstad, Petter (University of Bergen, Norway)
Brenner, Susanne (Louisiana State University, USA)
Cai, Xiao-Chuan (CU Boulder, USA)
Gander, Martin (University of Geneva, Switzerland, Chair)
Halpern, Laurence (Paris 13, France)
Keyes, David (KAUST, Saudi Arabia)
Kim, Hyea Hyun (Kyung Hee University, Korea)
Klawonn, Axel (Universität zu Köln, Germany)
Kornhuber, Ralf (Freie Universität Berlin, Germany)
Langer, Ulrich (University of Linz, Austria)
Quarteroni, Alfio (EPFL, Switzerland)
Widlund, Olof (Courant Institute, USA)
Xu, Jinchao (Penn State, USA)
Zou, Jun (Chinese University of Hong Kong, Hong Kong)

Local Organizing Committee

Ronald D. Haynes (Memorial University, Canada, Chair)
Scott MacLachlan (Memorial University, Canada)
Hermann Brunner (Hong Kong Baptist University, Hong Kong)
Sue Brenner (Louisiana State University, Baton Rouge, LA, United States)
Shaun Lui (University of Manitoba, Canada)
Emmanuual Lorin (Carleton University, Canada)
Heavy red or dark line shows a nice walking trail from Quidi Vidi lake to Memorial University along the Rennie Mills river.
Meeting registration in IIRC (Bruneau Centre for Innovation and Research), talks in IIRC and Arts and Admin (Arts for short!).
Arts First Floor (MS Rooms)
City Service List

City service:

PUBLIC TRANSPORTATION

METROBUS (www.metrobus.com)
Ride Guide
(Transit Info, 24 hours): 722-9400
Cash fare: Adult & Senior $2.25, Child $1.75
10-ride card: Adult $20, Senior & Child $15
Monthly pass: Adult $70, Senior & Child $45

TAXIS (These are probably the biggest companies)
Bugden’s Taxi: 722-4400
City Wide Taxi: 722-0003
Newfoundland Cabs: 744-4444
Jiffy Cabs: 722-2222
Red & Yellow Cabs: 726-6666

BANKS

BMO Bank of Montreal
384 Elizabeth Avenue
795-2110
Mon-Fri: 10 am - 5 pm

CIBC
Churchill Square (68-10 Rowan Street)
576-8777
Mon-Fri: 10 am - 5 pm

RBC Royal Bank
65 Elizabeth Avenue
576-4545
Mon-Fri: 9:30 am - 5 pm
Tues-Thurs: 9:30 am - 8 pm
ATM: University Centre

Scotia Bank
21 Elizabeth Avenue East
576-1988
Mon-Fri: 10 am - 5 pm
ATM: Science Building

TD Bank
80 Elizabeth Avenue
795-1850
Mon-Tues: 8 am - 6 pm
Wed-Fri: 8 am - 8 pm
Sat: 8 am - 4 pm

HEALTH SERVICES

The Sobeys and Dominion stores also contain pharmacies.

Blackmarsh Family Care Centre
(walk-in clinic)
260 Blackmarsh Road
576-6965
Mon-Fri: 9 am - 11:30 am, 1:30 pm - 4:30 pm, 6 pm - 9 pm
Sat, Sun: 9 am - 12 pm, 1 pm - 5 pm

Shoppers Drug Mart
394 Elizabeth Avenue
722-1500
Mon-Sun: 9 am - 10 pm

Lawtons Drugs
11 Elizabeth Avenue
722-3171
Mon-Sat: 9 am - 10 pm
Sun: 12 am - 10 pm

HOSPITALS

Health Science Centre
(General Hospital)
300 Prince Philip Drive
777-6300

St. Clare’s Mercy Hospital
154 LeMarchant Road
777-5000

GROCERY STORES

Colemans
129 Merrymeeting Road
576-3283
Mon-Sat: 8 am - 10 pm
Sun: 10 am - 6 pm

Dominion
20 Lake Avenue
576-1160
Sun-Mon: 8 am - 10 pm

Sobeys
8 Merrymeeting Road
726-2242
Mon-Sat: 8 am - 10 pm
Sun: 10 am - 6 pm

Sobeys
10 Elizabeth Avenue (Howley Estates)
753-3565
Mon-Thur: 8 am - 10 pm
Fri-Sat: 8 am - 11 pm
Sun: 10 am - 10 pm

RADIO STATIONS

VOCM 960 AM
CBC Radio 1 940 AM
VOWR 900 AM
Radio Newfoundland 930 AM
CHMR 93.5 FM
OZFM 94.7 FM
K-Rock 97.5 FM
Hits 99.1 FM
Coast 101.1 FM
KISS Country 103.9 FM
CBC Radio 2 106.9 FM
Food:

**On campus:**
- Bitters
- Field House
  - 884-3300
  - The graduate student pub. Easy to reach.
- Food Court
  - University Centre
  - A variety of food choices:
    - Mustang Sallys, Dairy Queen,
    - Booster Juice, Treats, Extreme Pita, Just Fries, Mr. Sub.
- Tim Hortons
  - Arts & Admin Bldg. First floor
- Tim Hortons
  - The Works Aquarena
  - 17 Westerland Road

**Near MUN:**
- East Side Mario's
  - 180 Portugal Cove Road
  - 722-6900
  - A pasta house; part of a national chain.
- Governor Pub and Eatery
  - 386 Elizabeth Avenue
  - 726-0092
  - Good pub food, and particularly great onion rings.
- The Pantry
  - Eline Dobbin Centre
  - 70 Clinch Crescent
  - 722-6200
  - Reservations are a MUST; a small cafe that is regularly full.
  - They do a very nice soup, salad, sandwich and dessert for lunch.
  - Proceeds go to the Autism Society of Newfoundland and Labrador.
- Fort Amherst Pub
  - 29 Rowan St.
  - Churchill Square
  - 746-4550
- NJ's Kitchen + Buffet
  - 15 Rowan St.
  - Churchill Square
  - (709) 257-4938
- Quintana's
  - Churchill Square
  - 579-7000
  - Nice Mexican food. They sometimes do a salsa sampler.
  - For a Big supper, try Montezuma's Revenge.
- Smithy's Restaurant
  - Terrace on the Square
  - Churchill Square
  - 576-0080
- The Rooms Cafe
  - 9 Bonaventure Avenue
  - 727-8597
  - This cafe is on the top floor of The Rooms, which also houses the Provincial Museum and Art Gallery.
  - A fantastic view comes with the meal. Binoculars are available at window seats. They are open daily for lunch, and evenings on Wednesday. Don't take reservations!
- Wedgewood Cafe
  - 17 Elizabeth Avenue
  - 726-1860
  - The permanent arm of a local catering company. Founded by Gordon Bleu-trained chef Peter Wedgewood.

**Downtown:**
- Bacaloes
  - 65 LeMarchant Rd
  - 579-0565
- Nouvelle Newfoundland Cuisine
- Bagel Cafe
  - 246 Duckworth Street
  - 739-4470
  - Known for their fantastic breakfast.
- Basho
  - 283 Duckworth Street
  - 576-4600
  - Japanese fusion; includes sushi.
- Blue
  - 319 Water Street
  - 754-2583
  - Fine (but expensive) supper dining. Very reasonably priced lunches.
- Boca Tapas Bar
  - 189 Water St.
  - 237-2622
- Celtic Hearth
  - 300 Water Street
  - 576-2880
  - Pub food 24 hours a day, but nice food from 4-11 p.m. Post George Street, this is the place to eat (unless you want a hot dog from a vendor).
- Chez's Fish and Chips
  - 9 Freshwater Road
  - 655 Topsail Road
  - 8 Highland Drive
  - 726-3434
  - THE place to go for classic fish and chips. Mention that you're from away to get a certificate proving you had the best fish and chips in Newfoundland.
- Chilindro Bistro
  - 5 Bates Hill, St. John's
  - 722-3100
- Coffee Matters
  - 1 Military Rd
  - 753-6980
  - Coffee shop across the street from the Sheraton Hotel.
- Get Stuffed
  - 190 Duckworth Street
  - 757-2480
  - A popular downtown restaurant.

More food choices next page!
Gypsy Tea Room
Murray Premises (5 Beck's Cove)
730-4766
A varied selection. A nice spot, with great ambiance and somewhat reasonably priced.

Hong Kong Restaurant
361 Water Street
753-8939
One of St. John's mainstays for Chinese food.

Magic Wok
408 Water Street
753-6907
A popular St. John's Chinese food restaurant. A big spot, reservations might still be needed.
(Mebo's) Press and Bean
291 Water St.
753-2457
Casual fine dining, if you can forgive the contradiction.

Merchant Tavern
291 Water St.
722-5050

Mochanopoly Board Game Cafe
204 Water St. St. John's
AIT 1A9
Hours: 3-11
(709) 574-3657

Oliver's
160 Water St.
754-6444
Contemporary neighbourhood eatery serving steaks, seafood & pasta with wine & local beers.

Pi
10 King's Road
726-2000
A gourmet pizza restaurant that is a MUST for any mathematician. How many places can you order a Fibonacci?

Platto Pizzeria Enoteca
60 Elizabeth Ave
(709) 726-0509
&
377 Duckworth St.
726-0909
Thin-crust wood fire pizza

Portobello's
115 Duckworth Street
579-7050
A classic grill with Italian influence.

Raymonds (one of the top restaurants in the country)
Classy place in a 1915 building with refined, locally sourced meals, wine pairings & a tasting menu.
95 Water St.
579-5900

Rocket Bakery & Fresh Food
272 Water St.
738-2015
Bright French-inspired bakery & cafe offering gourmet prepared foods for dine-in or takeout.

Sprout
364 Duckworth Street
579-5485
The single "vegetarian-only" restaurant in the city. Many vegan and gluten-free options as well.

St. John's Fish Exchange Kitchen & Wet Bar
351 Water St.
739-7599

Sun Sushi
186 Duckworth Street
726-8598
Besides being a popular sushi option, it's also the place for bubble tea.

Tavola Restaurant
178 Water St.
754-1678

The Adelaide Oyster House
334 Water St.
722-7222

Yellowbelly
288 Water Street
757-3764
A local brew pub with fine dining options.
Plenary Lecture Overview


Chair: Alfio Quarteroni

Plenary Lecture-01 David Keyes
8:30-9:15 Hierarchical Algorithms on Hierarchical Architectures

David Keyes

Chair: Martin J. Gander

Plenary Lecture-02 Hui Zhang
9:15-10:00 Unified Analysis of Iterative Methods Based on One-Way Domain Decomposition

Hui Zhang

Chair: David Keyes

Plenary Lecture-03 Martin J. Gander
2:00-2:45 On Scalability, Optimal and Optimized Coarse Spaces

Martin J. Gander

Tuesday, 24 July 2018  Venue: IIC-2001

Chair: Alison Malcolm

Plenary Lecture-04 Henri Calandra
8:30-9:15 A review of the computational aspects in Seismic Imaging and Reservoir Simulation

Henri Calandra

Chair: Laurence Halpern

Plenary Lecture-05 Claude Le Bris
9:15-10:00 Finite Elements Methods for multiscale problems, and related issues

Claude Le Bris

Chair: Olof Widlund

Plenary Lecture-06 Marcus Sarkis
8:30-9:15 Discretizations based on BDDC/FETI-DP Techniques

Marcus Sarkis

Chair: Jun Zou

Plenary Lecture-07 Zhiming Chen
9:15-10:00 Computation of High Frequency Waves in Unbounded Domains: Perfectly Matched Layer and Source Transfer

Zhiming Chen

Chair: Susanne Brenner

Plenary Lecture-08 Daniel Peterseim
2:00-2:45 Domain decomposition tips the scales: From additive Schwarz methods to homogenization

Daniel Peterseim

Thursday, 26 July 2018  Venue: IIC-2001

Chair: Petter Bjørstad

Plenary Lecture-09 Xiaoye (Sherry) Li
8:30-9:15 Reducing flops, communication and synchronization in sparse factorizations

Xiaoye (Sherry) Li

Chair: Scott MacLachlan

Plenary Lecture-10 André Fortin
9:15-10:00 Anisotropic mesh adaptation using enriched reconstructed solutions

André Fortin

Friday, 27 July 2018  Venue: IIC-2001

Chair: Axel Klawonn

Plenary Lecture-11 Matthew Knepley
8:30-9:15 Thoughts on Composing of Nonlinear Solvers

Matthew Knepley

Chair: Ulrich Langer

Plenary Lecture-12 Clemens Pechstein
9:15-10:00 An algebraic view on BDDC - from local estimates to eigenvalue problems, parallel sums and deluxe scaling

Clemens Pechstein
<table>
<thead>
<tr>
<th>Minisymposia</th>
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| **MS01**: Development of multilevel methods for coupled physics applications  
*Organizers: Adler, Hu, Zikatanov* |
| **MS02**: Solvers for nonstandard discretization methods: Theory and Applications  
*Organizers: Ayuso de Dios, Brenner, Sarkis* |
| **MS03**: Domain-decomposition methods for integral equation problems  
*Organizers: Ciaramella, Gander, Salomon* |
| **MS04**: Domain decomposition and model coupling issues for oceanic and atmospheric flows  
*Organizers: Tang, Blayo* |
| **MS05**: Reduced and adaptively enhanced coarse spaces and related multiscale discretizations  
*Organizers: Klawonn, Rheinbach, Widlund* |
| **MS06**: Extremely parallel domain decomposition methods and their applications  
*Organizers: Klawonn, Rheinbach* |
| **MS07**: Advances in algebraic multigrid  
*Organizer: Olson* |
| **MS08**: Domain Decomposition preconditioners for Isogeometric Analysis  
*Organizers: Pavarino, Widlund, Scacchi* |
| **MS09**: Fifty years of Domain Decomposition theory and algorithms: celebrating Olof B. Widlund’s 80th birthday  
*Organizers: Cai, Pavarino, Szyld* |
| **MS10**: Parallel-in-time methods for highly concurrent architectures  
*Organizers: Schroder, Falgout* |
Minisymposia cont’d

MS11: Parallel Methods for PDE-based Mesh Generation and Adaptation

Organizer: Shontz

MS12: Asynchronous Domain Decomposition Methods

Organizers: Boman, Szyld

MS13: Discretization and Multilevel Methods for Nonstandard FEM

Organizers: Pollock, Zhu

MS14: Transmission conditions in domain decomposition methods

Organizers: Halpern, Gander, Kwok

MS15: Advances in Schwarz waveform relaxation and space-time DD methods

Organizers: Kwok, Halpern, Gander

MS16: Solvers and preconditioners for non-conforming discretization methods

Organizers: Lucero, Gander

MS17: Domain Decomposition and Multilevel Methods for Wave Propagation

Organizers: Zhang, Gander

MS18: Probabilistic Domain Decomposition Methods

Organizers: Donzelli, Bihlo

MS19: Oil, Gas and Ocean Industry Session

Organizers: James, Malcolm, Haynes
Contributed Talks

Parareal algorithm for two phase flows simulation

K. Aït Ameur, Y. Maday, M. Tajchman

Patch-based finite element method for electromagnetic wave propagation problems in microwave discharge plasma

Emanuele Arcese*, François Rogier, Jean-Pierre Boeuf

Augmented Lagrangian domain decomposition method for a geological crack with friction

Amina Chorfi*, Olivier Bodart, Jonas Koko

An optimal control problem based on a fictitious domain method for inversion of the pressure contribution on the crack in the volcanic concepts

Oliver Bodart, Farshid Dabaghi*, Valérie Cayol, Jonas Koko

Convergence of classical and optimized Schwarz method for the 2-dimensional Maxwell’s equations with discontinuous coefficients and generalizations

Fabrizio Donzelli*, Alexander Biblo, Colin G. Farquharson, Martin J. Gander, Ronald D. Haynes

Multigrid Reduction in Time (MGRIT) for eddy current problems

Stephanie Friedhoff

Component-averaged DD: a parallel, problem-independent solution to the cross-point issue

Dan Gordon*, Rachel Gordon
Contributed Talks cont’d

Application of multilevel BDDC to incompressible Navier-Stokes equations

Martin Hanek

Local Fourier analysis of BDDC-like algorithms

Jed Brown, Yunhui He*, Scott MacLachlan

Asymptotic analysis for the coupling between subdomains in Discrete Fracture Matrix models

Martin J. Gander, Julian Hennicker*

A guaranteed nonlinearly preconditioned inexact Newton algorithm based on domain decomposition method

Jizu Huang

Theory and collocation solvers for integral-algebraic equations

Hui Liang*, Hermann Brunner

A nonlinearly preconditioned inexact Newton method for blood flow problems in patient-specific arteries with stenosis

Li Luo*, Wen-Shin Shiu, Rongliang Chen, Xiao-Chuan Cai

A hybrid transport-diffusion method for laser fusion simulation

Shuanggui Li*, Xudeng Hang, Jinghong Li

Schwarz methods for the implicit closest point method

Ian May*, Ronald D. Haynes, Steven Ruuth
Contributed Talks cont’d

A coupled acoustic-elastic wave solver for estimating seismic amplitudes

Ligia Elena Jaimes Osorio, Alison Malcolm*

A time adaptive multirate Neumann-Neumann waveform relaxation method for heterogeneous coupled heat equations

Azahar Monge*, Philipp Birken

Enabling physics-based domain decompositions in environmental applications through a flexible software ecosystem

J. David Moulton*, A. Jan E. T. Coon, S. L. Painter

A finite element nonoverlapping domain decomposition method with Lagrange multipliers for the dual total variation minimizations

Chang-Ock Lee, Jongho Park*

Instability-effects of a localization-method for nonlinearities in dual domain decompositions and use of recycling methods

Andreas S. Seibold*, Michael Leistner, Daniel J. Rixen

Conjugate gradient for nonsingular saddle-point systems with a highly singular leading block

Michael Wathen

A coupling simulation for the multilevel radiative diffusion equation based on the domain decomposition method

Rong Yang*, Xudeng Hang
Poster Session

Domain decomposition method for the Baltic Sea model based on theory of inverse problems and adjoint equation
Valery Agoshkov, Natalia Lezina

On the scalability of classical one level domain-decomposition methods
Faycal Chaouqui, Gabriele Ciaramella, Martin J. Gander, Tommaso Vanzan

Convergence of classical Schwarz method for the 2-dimensional Maxwell’s equations
Fabrizio Donzelli

Stability Analysis of Inline ZFP Compression for Floating-Point Data in Iterative Methods
Alyson Fox

SPMR: a Family of Saddle-Point Minimum Residual Solvers
Chen Greif

A new approach for preconditioning discontinuous Galerkin discretizations
Soheil Hajian

Domain decomposition method for the Baltic Sea model based on theory of inverse problems and adjoint equation
Natalia Lezina

A Reynolds Number Dependent Convergence Estimate for the Parareal Algorithm
Martin J. Gander, Thibaut Lunet

Domain Decomposition of Mixed Finite Element Method in ESPRESO
Lukas Maly
Poster Session cont’d

A generic framework for Schwarz decomposition methods

Pratik Nayak, Hartwig Anzt

Solving High-order Discretizations of Thermal Radiative Transport

Terry Haut, Peter Maginot, Ben Southworth, Vladimir Tomov

New Coarse Corrections for Optimized Restricted Additive Schwarz Using PETSc

Serge Van Criekingen, Martin J. Gander

Consensus Least-squares Reverse Time Migration

Toktam Zand, Ali Gholami, Alison Malcolm

Multilevel Optimized Schwarz Methods

Martin J. Gander, Tommaso Vanzan

A monotonicity preserving multigrid algorithm for solving the equidistributing meshes in 1D

Dawei Wang
### Overview of the Week

#### Monday, July 23, 2018

<table>
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<tr>
<th>Time</th>
<th>Arts-1045</th>
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<td>Opening - IIC 2001</td>
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#### Tuesday, July 24, 2018

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### Wednesday, July 25, 2018

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### Thursday, July 26, 2018

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### Friday, July 27, 2018

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Hierarchical Algorithms on Hierarchical Architectures

David Keyes*, Hatem Ltaief, and Stefano Zampini  George Turkiyyah  Rio Yokota

Some algorithms achieve optimal arithmetic complexity with low arithmetic intensity (flops/Byte), or possess high arithmetic intensity but lack optimal complexity, while some hierarchical algorithms, such as Fast Multipole and its H-matrix algebraic generalizations, realize a combination of optimal complexity and high intensity. Implemented with task-based dynamic runtime systems, such methods also have potential for relaxed synchrony, which is important for future energy-austere architectures, since there may be significant nonuniformity in processing rates of different cores even if task sizes can be controlled. We describe modules of KAUST’s Hierarchical Computations on Manycore Architectures (HiCMA) software toolkit that illustrate these features and are intended as building blocks of more sophisticated applications, such as matrix-free higher-order methods in optimization. HiCMA’s target is hierarchical algorithms on emerging architectures, which have hierarchies of their own that generally do not align well with those of the algorithm. Some modules of this open source project have been adopted in the software libraries of major vendors. We describe what is currently available, some motivating applications, and relevance to mainstream iterative methods for partial differential equations based on domain decomposition preconditioners.
Unified Analysis of Iterative Methods Based on One-Way Domain Decomposition for the Helmholtz Equation

Hui Zhang

Since the landmark paper Bjorn Engquist and Lexing Ying, Sweeping Preconditioner for the Helmholtz Equation: Moving Perfectly Matched Layers, 2011 (EY), we have seen a blossom of iterative methods based on one-way domain decomposition for the Helmholtz equation. All of them use PMLs or other high-order absorbing conditions on the subdomain boundaries as an essential ingredient. Many encouraging numerical results have appeared since the initiation by EY, and one observes a growing diversity in the development of new methods in this class such as the source transfer method, the single-layer potential method, the polarized traces method and the amplitude-preserving propagator method. They are based on various fascinating physical intuitions, which lead to apparently different formulations. Our quest begins with exploring how much different these methods are. Will one method perform better than the others due to what information is transferred between subdomains? Does it matter to take the volume variables, the residuals or certain traces as the iterates? If these methods converge similarly, is there a unique principle behind them? We will answer these questions in this talk. We first review two old algorithms: the block LU solver for a block tri-diagonal matrix and the optimal Schwarz method for second-order elliptic PDEs, followed by historical ideas for their approximate forms: the AILU preconditioners and the optimized Schwarz methods using absorbing conditions, and also using PMLs by Toselli in 1998 and Schädle and Zschiedrich in 2007. We then show that all these old/new algorithms before/after EY have equivalent iterates if the same absorbing conditions and overlaps are used. EY pivoted the first use of PMLs in block LU and first numerical evidence for challenging problems. By equivalence, we give a unified analysis of convergence. We finally present numerical difficulties that remain.
A Mixed-Method B-Field Finite-Element Formulation for Incompressible, Resistive Magnetohydrodynamics

James Adler*, Thomas Benson, Eric Cyr, Scott MacLachlan, Raymond Tuminaro

Magnetohydrodynamics (MHD) models describe a wide range of plasma physics applications, from thermonuclear fusion in tokamak reactors to astrophysical models. These models are characterized by a nonlinear system of partial differential equations in which the flow of the fluid strongly couples to the evolution of electromagnetic fields. As a result, the discrete linearized systems that arise in the numerical solution of these equations are generally difficult to solve, and require effective preconditioners to be developed. This talk investigates monolithic multigrid preconditioners for a one-fluid, viscoresistive MHD model in two dimensions that utilizes a second Lagrange multiplier added to Faraday’s law to enforce the divergence-free constraint on the magnetic field. We consider the extension of a well-known relaxation scheme from the fluid dynamics literature, Vanka relaxation, to this formulation. To isolate the relaxation scheme from the rest of the multigrid method, we utilize structured grids, geometric interpolation operators, Galerkin coarse grid operators, and inf-sup stable elements for both constraints in the system. Parallel numerical results are shown for the Hartmann flow problem, a standard test problem in MHD.

Robust Multilevel Preconditioners for a New Stabilized Discretization of the Poroelastic Equation

Peter Ohm*, James Adler, Francisco Gaspar, Xiaozhe Hu, Carmen Rodrigo, Ludmil Zikatanov

In this talk we present block preconditioners for a stabilized discretization of the poroelastic equations. The discretization is well-posed with respect to the physical and discretization parameters, and thus provides a framework to develop preconditioners that are robust with respect to such parameters as well. We construct these preconditioners for both the stabilized discretization and a perturbation of the stabilized discretization that leads to a sparser overall problem. We solve for the diagonal blocks of the preconditioners using multilevel methods. Numerical tests confirm the robustness of the block preconditioners with respect to the physical and discretization parameters.

Multilevel Preconditioners for Fractional Sobolev Spaces

Trygve Bærland*, Kent-Andre Mardal, Miroslav Kuchta

Coupled multiphysics problem often give rise to interface conditions best posed in fractional Sobolev spaces. Here, both positive- and negative fractionality are common. When designing efficient solvers for discretizations of such problems it would then be useful to have a preconditioner for the fractional Laplacian. In this work, we develop a parallel multigrid preconditioner for the fractional Laplacian with positive fractionality, and show a uniform bound on the condition number. For the case of negative fractionality, we give several preconditioning strategies. We finish with some numerical experiments verifying the theoretical findings.
Least square discretization and multilevel preconditioning for mixed variational formulations

Constantin Bacuta∗  Jacob Jacavage

We consider a least squares method for discretizing boundary value problems written as primal mixed variational formulations. For the mixed formulation we assume a stability LBB condition and a data compatibility condition at the continuous level. For the proposed discretization method a discrete inf − sup condition is automatically satisfied by the natural choices of test spaces (first) and the corresponding trial spaces (second). The discretization and the iterative approach does not require nodal bases for the trial space. We present a multilevel preconditioning approach that could take into considerations discontinuous coefficients and coupled physics of the problem to be solved. Immediate applications of the method include discretizations of second order PDEs with oscillatory or rough coefficients and first order systems of parametric PDEs, such as the time-hamonic Maxwell equations.

An Adaptive Domain Decomposition Method for DG discretization of an elliptic problem

Leszek Marcinkowski∗  Erik Eikeland  Talal Rahman

In this talk, we present an overlapping additive Schwarz method for a Discontinuous Galerkin discretization of second order elliptic problem in two dimensions, with highly varying coefficients. We propose variants of the adaptively built multiscale coarse space each containing local spaces spanned by functions constructed through solving specially defined eigenvalue problems over the 2D structures related to the interfaces between subdomains. The methods are easy to construct, inherently parallel, and overall effective. We present a theoretical bound for the condition number of the system, showing it is independent of the contrast in the coefficients when enough local eigenfunctions are added to the coarse space.

Adaptive Additive Average Schwarz Solvers for Hybrid Discontinuous Galerkin Discretizations

Yi Yu∗  Maksymilian Dryja  Marcus Sarkis

Additive Average Schwarz methods were introduced by Bjorstad, Dryja and Vainikko 97 and designed for solving 2D and 3D elliptic problems with discontinuous coefficients across subdomains using classical discretizations. The methods use no explicit overlap of the subdomains and the subdomain iteration is via the coarse space. The methods do not require a coarse triangulation, that is, one is free to choose arbitrary irregular subdomain. The coarse problem can be seen as inverting a low-rank perturbation of a diagonal matrix on the subdomain interfaces and so Sherman-Morrison-Woodbury formula can be used. The low-rank is equal to the number of subdomains and the numerical complexity per PCG iteration is:
one stiffness matrix-vector multiplication, one local problem per subdomain with zero Dirichlet data on the
subdomain interface, a global problem with one degree of freedom per subdomain and a diagonal scaling
on the degrees of freedom over the subdomain interfaces. The methods present several advantages with
respect to parallelization, startups and local and global solvers costs, specially in 3D, and they are algebraic
solvers. The condition number estimate of the preconditioned systems is of the same order as the classical
Additive Schwarz methods with minimum overlap and with a coarse space, that is, $O(H/h)$. In this talk
we design and analyze this type of preconditioning for Hybrid Discontinuous Garlekin discretizations with
heterogeneous coefficients, possibly with high-contrast coefficients and with the use of local generalized
eigenvalues problems in order to recover the robust $O(H/h)$ condition number estimate independently of
the coefficients.

**Nonoverlapping Schwarz method for hp-DGFEM with multiple penalty terms**

Piotr Krzyzanowski* Marcus Sarkis

For an elliptic second order PDE, we consider a symmetric interior penalty DGFEM discretization with
penalties applied not only to jumps of function values, but to fluxes as well [Douglas and Dupont, 1976],
[Arnold, 1982]. We analyze the preconditioning properties of a nonoverlapping, additive Schwarz method
with respect to the mesh size, polynomial order and penalty parameters.

**BDDC for incompressible Stokes with HDG**

Xuemin Tu* Bin Wang

A Balancing domain decomposition by constraints (BDDC) algorithm is studied for solutions of large sparse
linear algebraic systems arising from Stokes with hybridizable discontinuous galerkin (HDG) discretization.
The condition number for the preconditioned system is estimated and numerical results are provided to
confirm the results.

**A new coarse space correction for a well defined Neumann-Neumann method at the continuous level**

Fayçal Chaouqui* Martin J. Gander Kévin Santugini-Repiquet

The Neumann-Neumann domain decomposition preconditioner is well understood, and polylogarithmic
condition number estimates show its effectiveness for many elliptic problems. The method as a stationnary
iteration is however divergent, and not well posed at the continuous level when cross points are present in
the domain decomposition. While coarse space components are usually added to domain decomposition
methods to make them scalable, we propose here new coarse space components which permit to obtain a
well posed and convergent stationary two level Neumann-Neumann iteration in $H^2$, also in the presence
of cross points in the domain decomposition. We then show that the discretization of this new two level Neumann-Neumann method leads to effective preconditioners without logarithmic growth in the condition number.

**A Vertex Coarse Space for BDDC in Three Dimensions**

Clark R. Dohrmann* Kendall H. Pierson

We present a BDDC algorithm for three-dimensional scalar elliptic problems which uses a vertex coarse space. The basic idea is to replace the direct solver for a standard edge or face-based coarse problem by a preconditioner which requires much less computation and memory. The preconditioner employs a standard two-level additive Schwarz approach in which the coarse problem dimension equals the number of subdomain vertices and the local problems apply simple diagonal preconditioning. We show under certain assumptions that favorable BDDC condition number estimates for edge or face-based coarse spaces also hold for the proposed preconditioner. Numerical examples are presented to confirm the theory and to demonstrate the computational advantages of the approach. In closing, we discuss the current status of extending these ideas to elasticity in joint work with Olof Widlund.

**Multiscale Discretizations and Coarse Spaces Based on ACMS**

Alexander Heinlein* Axel Klawonn Jascha Knepper Oliver Rheinbach

Multiscale discretizations as well as coarse spaces for domain decomposition methods can be enhanced by incorporating basis functions computed from generalized eigenvalue problems. In particular, when solving problems with large variations in the coefficients, this enhancement is crucial to ensure robustness of the methods. The Approximate Component Mode Synthesis (ACMS) multiscale discretization extends the Multiscale Finite Element Method (MsFEM) by eigenfunctions of local generalized eigenvalue problems on interface components, i.e., edges and, in three dimensions, faces. The ACMS eigenfunctions are similar to coarse basis functions typically used in adaptive domain decomposition methods, and indeed, slight modifications of the eigenvalue problems lead to coarse spaces for two-level Schwarz methods that are robust with respect to variations in the coefficients. The eigenvalue problems use local Schur complements and replace Poincaré inequalities to obtain a condition number bound which depends on a user-defined threshold but does not depend on the contrast of the coefficients anymore. In this talk, the ACMS method and ACMS coarse space are extended to three dimensions, and numerical results for different model problems, including unstructured domain decompositions, are presented.

**Machine Learning in adaptive domain decomposition methods – predicting the geometric location of constraints**

Alexander Heinlein Axel Klawonn* Martin Lanser Janine Weber

The convergence rate of domain decomposition methods is generally determined by the eigenvalues of the preconditioned system. For second-order elliptic partial differential equations, coefficient discontinuities with a large contrast can lead to a deterioration of the convergence rate. A remedy can be obtained by enhancing the coarse space with elements, which are often called constraints, that are computed by solving small eigenvalue problems on portions of the interface of the domain decomposition, i.e., edges in two dimensions or faces and edges in three dimensions. In the present work, without restriction of generality, the focus is on two dimensions. In general, it is difficult to predict where these constraints
have to be computed, i.e., on which edges. Here, a machine learning based strategy using neural networks is suggested to predict the geometric location of these edges in a preprocessing step. This reduces the number of eigenvalue problems that have to be solved during the iteration. Numerical experiments for model problems and realistic microsections using regular decompositions as well as those from graph partitioners are provided, showing very promising results.

Chair: Martin J. Gander

10:30-12:30

MS17: Domain Decomposition and Multilevel Methods for Wave Propagation

Fast Low Rank Methods for Frequency Domain Wave Propagation

Björn Engquist*

We will discuss two aspects of large-scale simulation of high frequency wave propagation in frequency domain. One is the development and analysis of efficient sweeping type preconditioners based on low rank approximation. The application is numerical algorithms of near optimal computational complexity for certain variable coefficient differential equations. The other aspect is analysis revealing when algorithms of this type of operator low rank compression are possible and when they are not. This analysis is based on decorrelation estimates related to kernels of Helmholtz type.

An accurate, fast, and scalable solver for high-frequency wave propagation

Leonardo Zepeda-Núñez*  Matthias Taus  Russell Hewett  Laurent Demanet

In many science and engineering applications, solving time-harmonic high-frequency wave propagation problems quickly and accurately is of paramount importance and historically challenging. For example, in geophysics, such problems can be the forward problem in an iterative process for solving the inverse problem of subsurface inversion. It is crucial to solve these wave propagation problems accurately in order to obtain meaningful solutions. Additionally, due to the iterative nature of most optimization algorithms, the forward problem must be solved many times. Therefore, a fast solver is necessary to make solving the inverse problem feasible.

Recently, there have been many fast solvers have been developed for such problems. While most methods scale optimally only in the context of low-order discretizations and smooth wave speeds, the method of polarized traces has been empirically shown to retain optimal scaling for high-order discretizations, such as hybridizable discontinuous Galerkin methods, and for highly heterogeneous wave speeds, making it highly attractive for geophysical applications.

In this work, we introduce a new version of the method of polarized traces which reveals more parallel structure than previous versions while preserving all of its other advantages.

Non-Overlapping Domain Decomposition Algorithm Using Quasi-Optimal Transmission Conditions for the Helmholtz Equation

Yassine Boubendir
In this talk, we review a non-overlapping domain decomposition algorithm based on the so-called quasi-optimal transmission conditions in a context of a finite element approximation approach. We describe a modification of this algorithm that delivers similar convergence results with a reduced computational cost in particular in the three-dimensional case. In addition, we present some new extensions of this algorithm coupling accurate absorbing boundary conditions and using the cross-points technique introduced in the past for nodal finite elements. Numerical results validating these new methods are presented.

Enabling numerically exact local solver for waveform inversion— a low-rank approach

Rajiv Kumar  Bram Willemsen  Alison Malcolm*

Large scale full-waveform inversion involving partial differential equations (PDEs) is an expensive process to estimate the physical parameters of the subsurface where the main computational bottleneck is solving the PDEs in a large domain. Simulating wavefields in the entire domain is costly and can result in slower convergence, specially for time-lapse seismic monitoring, where the area of interest is around reservoir. To overcome this, numerically exact local-solver is proposed that accurately compute the wave-equations within area of interest which are, to machine precision, identical to those generated by a full-domain solver evaluated within the region of interest. Although, the local-solver can drastically reduce the computational cost and improve the convergence of waveform inversion, it requires the computation of the Green’s function in the background model at the surface and at the boundary of the local domain. This is prohibitively computationally demanding operation for large-scale 3D seismic data acquisition. In this work, we will consider a linear algebra approach to deal with the low-rank representation of the fully sampled Green’s function. Using complicated geological structures, we show that we do not have to simulate full Green’s function but get actions of it on well-chosen probing vectors, based on Low-Rank decomposition or randomized SVD. This representation allows us to have access to all the Green’s function at the surface and at the boundary of the local domain, and it can significantly reduce the computational bottleneck of simulating the Green’s function in the background model.
Parareal algorithm for two phase flows simulation

K. Aït Ameur*  Y. Maday  M. Tajchman

In the nuclear energy domain, system codes are dedicated to the thermal-hydraulics analysis of nuclear reactors for safety studies. We are here interested in the Cathare code developed by CEA, EDF, AREVA-NP and IRSN. Cathare solves the 6-equations/two-fluid model by considering a set of conservation laws (mass, momentum and energy) for each phase liquid and vapor. The discretization is based on a finite volume method on staggered grid in space and on a fully implicit time integration method. Typical cases involve up to a million of numerical time iterations, computing the approximate solution during long physical simulation times. On the other hand, the discretization level is kept intentionally at a coarse level to be able to handle whole systems simulations. Cathare is used in a simulator of a reactor submitted to accidental events. This platform is dedicated to train operators and prepare crisis management exercises thus requiring real-time response of the code. To optimize the response time, we consider a strategy of time domain decomposition, complementing the current space domain decomposition. This strategy is based on the parareal method, introduced in [G. Turinici, J.-L. Lions, Y. Maday. Résolution par un schéma en temps “pararéel”. 2001], that provides a strategy for “parallel-in-time” computations and offers the potential for an increased level of parallelism. Here we apply the parareal algorithm to the resolution of an oscillating manometer. This test case is proposed in [N. Zuber, G.F. Hewitt, J.M. Delhaye. Multiphase science and technology, volume 6. 1991] for system codes to test the ability of each numerical scheme to preserve system mass and to retain the gas-liquid interface. Since the Cathare time scheme is a multi-step scheme, we study how to adapt the parareal algorithm to this characteristic (analog to [S. Volz, C. Audouze, M. Massot. Symplectic multi-time step parareal algorithms applied to molecular dynamics, 2009]) and to validate it with an advection-diffusion equation solved with a Leapfrog scheme.

Patch-based finite element method for electromagnetic wave propagation problems in microwave discharge plasma

Emanuele Arcese*  François Rogier  Jean-Pierre Boeuf

Plasma dynamics during microwave gas breakdown has been extensively studied during the last decades. Numerical modeling of the strong mutual interaction of high frequency electromagnetic waves and plasma is inherently challenging due to the disparate spatial and temporal scales involved. In this talk, we present a finite element domain decomposition method with complete overlapping using a multi-scale approach, first introduced in [R. Glowinski, J. He, A. Lozinski, J. Rappaz et J. Wagner. Finite element approximation of multi-scale elliptic problems using patches of elements, Numerische Mathematik, 101 (4), pp. 663–687 (2005)], for numerically solving problems of electromagnetic wave propagation in a conducting medium such as plasma arising in microwave plasma discharge modeling. The problem consists of time-domain Maxwell’s equations coupled with plasma transport equations via the time-varying electron current density [E. Arcese, F. Rogier, J.P. Boeuf, Plasma fluid modeling of microwave streamers : approximations and accuracy, Physics of Plasmas, 24 (11): 113517 (2017)]. The proposed method addresses the treatment of electromagnetic fields by solving the problem successively on a coarse mesh covering the whole computational domain and on a single or multiple local “patches” with finer meshes, corresponding to plasma location, through a flexible multiplicative Schwarz algorithm. A spectral mixed finite element formulation
is adopted for the spatial discretization of the coupled wave propagation equations. Regarding time integration, an explicit leapfrog time-stepping technique is implemented in order to obtain a fast multi-level resolution algorithm. Its stability is thus ensured through an energy estimate. This patch-based method is applied and validated in two dimensional microwave breakdown in air and numerical examples are shown to illustrate its computational efficiency and accuracy with respect to the standard Yee’s scheme.

Augmented Lagrangian domain decomposition method for a geological crack with friction

Amina Chorfi*  Olivier Bodart  Jonas Koko

The reduction of the computational cost of solutions is a key issue to crack identification or crack propagation. One of the solution is to avoid re-meshing the domain when the crack moves by using a fictitious domain method [O. Bodart, V. Cayol, S. Court and J. Koko, XFEM-based fictitious domain method for linear elasticity with crack. SIAM Journal Scientific Computing 38, 219-246, 2016]. We consider a geological crack in which the sides do not pull apart. To avoid re-meshing, we propose an approach combining the finite element method, the fictitious domain method and the augmented Lagrangian method. We first extend artificially the crack to split the domain into subdomains with

- prescribed homogeneous normal displacement jump condition on the crack;
- prescribed homogeneous displacement jump condition on the extended fictitious crack.

We then introduce an auxiliary unknown to ensure the splitting of the differentiable part of the problem (linear elasticity) and the non differentiable part (friction term). We obtain a convex linearly constrained minimization problem with a nondifferentiable cost function. Using the augmented Lagrangian functional [R. Glowinski and P. Le Tallec, Augmented Lagrangian and Operator-splitting Methods in Nonlinear Mechanics, SIAM Studies in Applied Mathematics, Philadelphia, USA, 1989], we derive an Alternating Direction Method of Multiplier (ADMM) domain decomposition method. Numerical experiments are carried out to illustrate the applicability of the proposed method.

12:30-2:00 Lunch Break

Chair: David Keyes

2:00-2:45 Plenary Lecture-03 Martin J. Gander IIC-2001

On Scalability, Optimal and Optimized Coarse Spaces

Martin J. Gander*

It is well accepted in our community that domain decomposition methods need coarse space corrections to be scalable, and for all classical domain decomposition methods like Schwarz, Dirichlet-Neumann, Neumann-Neumann and FETI methods there are rigorous proofs of this. There are however also observations of scalability of domain decomposition methods without coarse space corrections, and scalability can depend on the nature of the PDE, the geometry and, maybe surprisingly, the boundary conditions. I will first review situations in which classical one level domain decomposition methods are scalable. I will then introduce for situations where the methods are not scalable a so called optimal coarse space.
This is a coarse space in which one can compute a coarse space correction which makes the underlying domain decomposition method converge in one iteration, i.e. we obtain a direct solver. The optimal coarse space naturally depends on the domain decomposition method used, and shows that a coarse space can do much more than just provide scalability, it can also fix flaws of the underlying domain decomposition method. The optimal coarse space is however in general very high dimensional, and to obtain a practical coarse space correction, I will then show how to choose an approximation of the optimal coarse space in an optimized way, leading to the fastest convergence possible for a given dimensionality of the coarse space. This choice also depends on the domain decomposition method used, and sheds new light on the recent field of coarse space development for multiscale and high contrast problems. I will finally show a convergence result using the abstract Schwarz framework for a two level additive Schwarz method with optimized coarse space applied to multiscale problems.
Convergence Analysis of the Full Approximation Scheme for Nonlinear Problems

Xiaozhe Hu* Long Chen Steven Wise

The Full Approximation Scheme (FAS) is a variant of multigrid methods, which has mainly been used for solving nonlinear problems but also has many other applications. Although the FAS achieves good performance in practice, its convergence theory is not well understood. In this talk, we view the FAS as an inexact successive subspace optimization method and show that the FAS converges uniformly under the standard assumptions on the objective function and space decomposition.

Algebraic Multigrid for Directed Graph Laplacian Linear Systems (NS-LAMG)

Alyson Fox* Thomas Manteuffel

Often real-world graphs are directed, meaning that information flows from a vertex to another vertex in one direction, such as hyperlink graphs, biological neural networks and electrical power grids. There are many applications where data scientists are interested in solving linear systems associated with directed graphs. Currently, data scientists are using preconditioned GMRES and Bi-CG to solve linear systems involving directed graph associated matrix representations (e.g. graph Laplacian). However, these methods tend to be unacceptably slow as the number of edges grows. We propose nonsymmetric lean algebraic multigrid (NS-LAMG), a new algebraic multigrid algorithm for directed graph Laplacian systems that combines ideas from undirected graph Laplacian multigrid solvers and multigrid algorithms for Markov chain stationary distribution systems. Low-degree elimination, proposed in LAMG for undirected graphs, is generalized to directed graphs and is a key component of NS-LAMG. In the setup phase, we propose a simple stationary-aggregation multigrid algorithms for Markov chain stationary distribution systems solver enhanced by low-degree elimination to find the right null-space vector that is used for the intergrid transfer operators. Numerical results show that low-degree elimination improves performance and that NS-LAMG outperforms GMRES for real-world, directed graph Laplacian linear systems.

Preconditioning mixed finite element discretizations for the Richards equation

Juan Batista* Ludmil Zikatanov

We present a method for simulating flow in unsaturated media based on a mixed finite element discretization for the time transient Richards’ equation. We discretize the problem using $RT_0 - P_0$ mixed finite element pair and we consider several linearization techniques for this nonlinear equation. The resulting linear systems are non-symmetric in general and their preconditioning could be a challenge, especially in cases with large variations in the diffusion. We design a preconditioner using primal discretization of an auxiliary, linear convection-diffusion equation. To efficiently solve the linear system we use a multilevel method based on ordered Gauss-Seidel smoother and unsmoothed aggregation coarsening. We present several numerical examples and report on the convergence of the different choices of linearizations as well as on the efficacy of the preconditioner. This work is in collaboration with L. Zikatanov (Penn State), X. Hu (Tufts), and James Adler (Tufts).
Generalized Bootstrap AMG

James Brannick

This talk focuses on developing a generalized bootstrap algebraic multigrid algorithm for solving sparse matrix equations. As a motivation of the proposed generalization, we consider an optimal form of classical algebraic multigrid interpolation that has as columns eigenvectors with small eigenvalues of the generalized eigen-problem involving the system matrix and symmetrized smoother. We use this optimal form to design an algorithm for choosing and analyzing the suitability of the coarse grid. In addition, it provides insights into the design of the bootstrap algebraic multigrid setup algorithm that we propose, which uses as a main tool a multilevel eigensolver to compute approximations to these eigenvectors. A notable feature of the approach is that it allows for general block smoothers and, as such, is well suited for systems of partial differential equations. In addition, we combine the GAMG setup algorithm with a least-angle regression coarsening scheme that uses local regression to improve the choice of the coarse variables. These new algorithms and their performance are illustrated numerically for scalar diffusion problems with highly varying (discontinuous) diffusion coefficient and for the linear elasticity system of partial differential equations.

Chair: Hui Zhang

3:15-5:15 MS17: Domain Decomposition and Multilevel Methods for Wave Propagation

Multiscale modeling of transient electromagnetic fields in highly heterogeneous media

Luz Angélica Caudillo-Mata* Eldad Haber

Efficient and accurate simulation of transient electromagnetic responses of geologically-rich geophysical settings is crucial in a variety of scenarios, including mineral and petroleum exploration, water resource utilizations and geothermal power extractions. In this talk, we develop a multiscale method to compute such type of responses in a very effective manner. Geophysical time-varying electromagnetic simulations of highly heterogeneous media are computationally expensive. One major reason for this is the fact that very fine meshes are often required to accurately discretize the physical properties of the media, which may vary over a wide range of spatial scales and several orders of magnitude. Using very fine meshes for the discrete models lead to solve large systems of equations that are often difficult to deal with at each time step. To reduce the computational cost of the electromagnetic simulation, we develop a multiscale method for the quasi-static Maxwell’s equations in the time domain. Our method begins by locally computing multiscale basis functions at each time step, which incorporate the small-scale information contained in the physical properties of the media. Using a Galerkin proper orthogonal decomposition approach, the local basis functions are used to represent the solution on a coarse mesh. The governing equations are numerically integrated using an implicit time marching scheme. Our approach leads to a significant reduction in the size of the final system of equations to be solved and in the amount of computational time of the simulation, while accurately approximating the behavior of the fine-mesh solutions. We demonstrate the performance of our method in the context of a geophysical electromagnetic application.
Scalable convergence using two-level deflation preconditioning for the Helmholtz equation

Vandana Dwarka∗ Cornelis Vuik

Recently, the use of deflation techniques has become popular to improve the convergence of iterative Helmholtz solvers. It is utilized to boost the performance of the Complex Shifted Laplacian Preconditioner (CSLP), as the eigenvalues of the preconditioned system shift towards the origin as the wave number increases. The two-level-deflation preconditioner combined with CSLP (ADEF) showed encouraging results in moderating the rate at which the eigenvalues approach the origin. However, for large wave numbers the initial problem resurfaces and the near-zero eigenvalues reappear. Our research sheds light on the cause of these reappearing eigenvalues and proposes the use of higher-order approximation schemes to construct the deflation vectors. The main effect of using a higher-order scheme is that the near-singular eigenmodes of the fine-grid and coarse-grid operator remain aligned during intergrid transfer operations. The results from Rigorous Fourier Analysis (RFA) and numerical experiments confirm that our newly proposed scheme outperforms any deflation-based preconditioner for the Helmholtz problem. In particular, the spectrum of the adjusted preconditioned operator stays fixed near one. For the first time, the convergence properties for very large wavenumbers ($k = 10^6$ in one-dimension and $k = 1500$ in two-dimensions) have been studied, and the convergence is close to wave number independence. The new scheme additionally shows very promising results for the more challenging Marmousi problem.

A finite difference method with optimized dispersion correction for the Helmholtz equation

Xueshuang Xiang Pierre-Henri Cocquet Martin J. Gander*

We develop a new dispersion minimizing FDM for the 2D Helmholtz equation using as a new idea a modified wave number. The talk will start from the modified wave number for the 1D Helmholtz equation, with a focus on the discontinuous coefficient case. For the 2D Helmholtz equation, compared with the finite difference scheme which minimizes already the numerical dispersion, our new scheme using the same stencil, but a modified wave number, has substantially less dispersion error and thus much more accurate phase speed, which is important for effective coarse grid corrections in domain decomposition and for constructing efficient multigrid solvers. The numerical examples indicate that for plane wave solutions, the new FDM is sixth-order accurate.

A finite difference method with reduced numerical dispersion for the Helmholtz equation

Pierre-Henri Cocquet

Solving the Helmholtz equation with iterative methods is very challenging for instance due to its indefinite nature or highly oscillatory solutions. In addition, the wave number associated to the numerical solution is different from the one of the exact solution thus leading to so-called numerical dispersion which requires very fine mesh to be controlled.

It has been shown in [Ernst, O. G., & Gander, M. J. (2013). Direct and Inverse Problems in Wave Propagation and Applications, 14.] that the numerical dispersion can be suppressed in 1d by using a standard 3-point stencil with a modified wavenumber. The latter is based on the fact that the discrete and continuous dispersion relation can be matched in 1D and thus this method can not be extended directly.
to higher dimensional problems. In this talk, we will study a similar approach for a finite difference method in 2d. We are going to use a 9-point stencil whose free-parameters can be optimized to reduce the numerical dispersion by minimizing the distance between the discrete and continuous dispersion relation. Our results are numerical, but we also provide analytical formulas for the optimized parameters and modified wavenumber indicating that the numerical dispersion can be greatly reduced even for a number of grid points per wavelength that is above the threshold required for accurate simulation of wave propagation. This presentation includes joint work and work in progress with Martin J. Gander and Xueshuang Xiang.

Chair: Alex Bihlo

3:15-5:15
MS18:Probabilistic Domain Decomposition Methods
Arts-1043

Recent advances on the numerics of stochastic representations to boundary-value problems

Francisco Bernal

A critical ingredient in Probabilistic Domain Decomposition (PDD) is the efficient numerical approximation, in terms of the computational complexity required to attain a preset accuracy (within a preset confidence interval), of the Feynman-Kac and related formulas. In this talk, I will give a survey of recent advances in the numerical integration of stochastic differential equations which are spatially bounded by a closed surface, which can be partially reflecting and partially absorbing. Such schemes allow for the pointwise solution of general boundary value problems with mixed boundary conditions. In particular, I will discuss the following novel strategies in which I have been involved: variance reduction based on pathwise control variates; a Multilevel strategy with linear variance decay across the levels; an implementation of Milstein’s walk on ellipsoids method; and a strategy to deal with boundary singularities typical of mixed boundary conditions. The talk will mostly skip technical details and focus on the ideas, difficulties, and experimental results.

2D Winslow Mesh Generation: general theory and stochastic solution

Fabrizio Donzelli* Oleksandr Abramov Alexander Bihlo Ronald D. Haynes

The mesh generation proposed by Winslow is given by a transformation \((x,y) \rightarrow (\xi, \eta)\) from the physical domain to the computational domain, where \(\xi\) and \(\eta\) are solution of the Laplace equation \(\nabla(w\nabla u) = 0\). The positive function \(w\) is called mesh density function and it can be interpreted as a metric on the physical domain. More generally, we can realize \(\xi\) and \(\eta\) as harmonic maps with respect to given metric on the physical and computational domain. In this talk we first prove, using a remarkable result of the theory of harmonic map, that the map \((x,y) \rightarrow (\xi, \eta)\) is a diffeomorphism between the physical and the computational domain. We then present a stochastic construction of the solutions \(\xi\) and \(\eta\) based on the Feynmann-Kac formula, which will be used, as presented in the talk of O. Abramov, to provide a stochastic domain decomposition solution of the WMG equations.

Parallelization of variational mesh adaptation based on Winslow method

Oleksandr Abramov* Alexander Bihlo Fabrizio Donzelli Ronald D. Haynes

Adaptive meshes appear to be preferable to the uniform meshes for some classes of numerical problems. As
a solution of numerical problems often involves solving a problem on a distributed computational systems (clusters), it is desirable for a mesh adaptation method to also work on such systems. An implementation of a library for a parallel adaptive moving mesh method based on Winslow method will be presented. The library is written on C++ language and uses a PETSc library and Message Passing Interface (MPI) protocol. Also an example of using the library with a stochastic domain decomposition based on Monte Carlo method will be discussed with some numerical results provided.

**Domain Decomposition of Stochastic PDE - New Developments**

Abhijit Sarkar∗ Ajit Desai Mohammad Khalil Chris Pettit Dominique Poirel

In the framework of intrusive spectral stochastic finite element method, the mathematical formulations and associated scalability studies of two-level non-overlapping domain decomposition (DD) solvers are reported in [1, 2, 3, 4] for stochastic partial differential equations (SPDEs). While the scalability results (for a few random variables) of these two-level DD solvers, based on vertex-based coarse grids, are promising for two-dimensional scalar SPDEs, the performance of these algorithms degrades for three-dimensional coupled SPDE systems, for instance, arising in the linear elasticity. The poor scaling of these algorithms for coupled three-dimensional SPDE systems can be attributed to the geometrical complexities of the global interface, complicated spatial coupling among subdomains in conjunction with the additional block coupling structure along the stochastic dimension in the intrusive polynomial chaos approach. To address this difficulty, a probabilistic version of a wirebasket preconditioner (having enriched coarse grid) is proposed which improves the performance of the previous two-level domain decomposition solvers having only the vertex-based coarse grid correction. Additionally, the computational advantages of the two-level intrusive domain decomposition solvers are demonstrated in handling large number of random variables, compared to the sparse grid quadrature based non-intrusive solvers.

**An optimal control problem based on a fictitious domain method for inversion of the pressure contribution on the crack in the volcanic concepts**

Oliver Bodart Farshid Dabaghi∗ Valérie Cayol Jonas Koko

We study an inversion of a pressure contribution parameter on the fracture inside a volcano by a fictitious domain method. We begin by the domain decomposition of an elastic body into two sub-domains by using an artificial extension of the considered crack. The crack and its extension are represented by level-set functions. Then, an optimal control formulation, by using a Lagrangian involving a cost function, a smoothing part, and the weak formulation of the physical problem is introduced. Finally, numerical experiments with the realistic volcanic data, highlights the applicability of the method.

**Multigrid Reduction in Time (MGRIT) for eddy current problems**

Stephanie Friedhoff
Maxwell’s equations are an essential tool in the numerical simulation of problems in electrical engineering. A standard approach for the simulation of electrical machines is to neglect the displacement current in Maxwell’s equations, yielding the so-called magnetoquasistatic approximation or, synonymously, the eddy current problem. Typically, solution algorithms for the time-dependent eddy current problem are based on a time-marching approach, solving sequentially for one time step after the other. The computational complexity of such approaches is high, particularly if long time periods have to be considered as, for example, in the case of simulating the start-up of an electrical machine. One approach for reducing the simulation time is with parallel-in-time integration techniques as shown in [S. Schoeps, I. Niyonzima, and M. Clemens, Parallel-in-Time Simulation of Eddy Current Problems using Parareal, 21st Conference on Computation of Electromagnetic Fields (COMPUMAG 2017), Daejeon, Korea, June 2017] for the Parareal algorithm [J.-L. Lions, Y. Maday, and G. Turinici, A "parareal" in time discretization of PDEs, C. R. Acad. Sci. 332 (2001), pp. 661-668]. In this talk, we consider Multigrid Reduction in Time [R. D. Falgout, S. Friedhoff, Tz. V. Kolev, S. P. MacLachlan, and J. B. Schroder, Parallel time integration with multigrid, SIAM J. Sci. Comput. 36 (6), pp. C635-C661] for the time-parallel solution of the eddy current problem. In particular, we present numerical results for a 2D model problem of a conducting wire surrounded by a pipe.

Component-averaged DD: a parallel, problem-independent solution to the cross-point issue

Dan Gordon∗ Rachel Gordon

A major issue in domain decomposition (DD) is that of eliminating problems caused by integrating the subdomain solutions across subdomain boundaries. An even harder problem arises in the case of cross points, at which three or more subdomains meet. This topic has received a lot of attention in recent years, with several problem-specific solutions. It is shown that these problems do not exist with the block-parallel CARP-CG algorithm [G & G, PARCO 2010], which is the prototype of component-averaged domain decomposition (CADD). This is due to the fact that in CARP-CG, both the local processing and the merging of the local solutions are, in effect, solved in a certain superspace in a unified manner. Furthermore, there is no need for any problem-specific adaptation. In CADD, the domain is partitioned by boundaries passing between grid points. Every grid point next to a subdomain boundary is cloned in the processor(s) operating on adjacent subdomain(s), and the clones are treated as if they were the actual grid points. After the parallel processing of the subdomains, every boundary grid point and its clones are averaged and redistributed to the neighboring subdomains. In CARP-CG, the interior algorithm is Kaczmarz and the averaging is equivalent to Kaczmarz projections in a superspace, so an external CG can be used to accelerate the process. CARP-CG is particularly efficient for problems with very large off-diagonal elements and/or discontinuous coefficients, such as convection-dominated PDEs and high-frequency Helmholtz equations.

Application of multilevel BDDC to incompressible Navier-Stokes equations

Martin Hanek

We deal with numerical simulation of incompressible flows using multilevel Balancing Domain Decomposition based on Constraints (BDDC). We apply this method to non-symmetric problems arising from the linearized incompressible Navier-Stokes equations. Picard iteration is used for linearization, and the arising linear system is solved by the BiCGstab method using one step of BDDC as a preconditioner. The multilevel BDDC method is applied to a benchmark problem of 3-D lid-driven cavity and to an industrial problem of oil flow in hydrostatic bearing.
5:15– Free Time
A review of the computational aspects in Seismic Imaging and Reservoir Simulation

Henri Calandra

For several decades, the Oil and Gas industry has been committed to produce more and more hydrocarbons in response to the growing world demand for energy. Always seeking deeper and farther, exploration and development has become economically challenging as a result of increased geological and above ground complexity, stronger environmental constraints and pressure on costs. Progress in data acquisition, rapid progress in rocks physics labs, more powerful computers and integrated teams including physicists and computational scientists have greatly contributed to the development of advanced numerical algorithms integrating more and more complex physics and delivering high value to the O&G industry. HPC modeling and simulation is a leading technology in this effort. Faster algorithms and hardware lead to improved “visibility” of the subsurface and the systematic investigation of more drilling and production scenarios. The vast amounts of seismic data recorded on the fields are explored using imaging algorithms to illuminate the hidden subsurface of the earth, and reservoir simulation is used to optimally produce fields and predict the time evolution of the assets. The industry is evolving on several fronts. Changes in the underlying hardware with the advent of new technologies are challenging practitioners to develop new algorithms. Seismic imaging and reservoir simulation rely on different physics, governed by different PDEs. Solving those PDEs is done through a large range of numerical approximations such as finite differences, finite element continuous or discontinuous Galerkin, finite volume for the spatial derivatives, explicit time integration, implicit time integration, mixed explicit-implicit for integrating the time. The choice of the numerical methods and the time integration is very dependent on the nature of the problem to be solved. Explicit time marching methods for solving wave equations in seismic and finite difference spatial discretization are the most popular and are very efficient for seismic depth imaging. Fully implicit or mixed implicit-explicit
combined with finite volume methods are today the standard for reservoir simulation. Numerical approximations have an important impact on model representation: centered grid, staggered grid, rotated grid, meshes (tetrahedron, hexahedron), cells, etc. Corresponding implementations on modern computers are also very dependent on the nature of the problem to be solved. A very high efficiency and scalability can be reached for seismic depth imaging algorithms. Seismic depth imaging is embarrassingly parallel in the shot profile dimension. Numerical kernels are very well adapted to take advantage of modern compute nodes such as multicores CPUs and accelerator technologies. Parallel implementations over large distributed memory computers are based on spatial domain decomposition. In this case load balancing and ghost communication across sub-domains are the main bottlenecks to be addressed. Reservoir simulation solves the nonlinear system of equations that links the different reservoir parameters. The method is a classic Newton-Raphson method with some modifications specific to reservoir simulation. Each iteration of the Newton method requires the solution a linear system that is a linearization of the non-linear function. The computational effort of the linear solver represents up to 80-90% of the overall simulation time. In reservoir simulation, efficiency is very dependent on the linear solver scalability and efficiency, and an important R&D effort is spent on the definition and implementation of scalable solvers. The first part of this talk introduces the challenging environment of the O&G industry and demonstrates the value that numerical simulation combined with the progress of HPC and other technologies have delivered to our industry. The second part will present some of the computational aspects in seismic depth imaging and reservoir simulation and the important effort spent on more advanced numerical methods and algorithm design, improving numerical solutions and taking advantage of the fast evolution of HPC technology.

Chair: Laurence Halpern

9:15-10:00 Plenary Lecture-05 Claude Le Bris IIC-2001

Finite Elements Methods for multiscale problems, and related issues.

Claude Le Bris*

The talk will overview some recent contributions to the mathematical theory and the development of multiscale finite element methods, in particular with applications to non periodic media. The approaches described aim at capturing the fine scale structure of the solution to an elliptic oscillatory equation while using a coarse mesh. To this end, the basis functions are adjusted to the problem under consideration, and precomputed on a finer mesh using the so-called local problems, reminiscent of the corrector problem of homogenization theory. Various issues arise, both at the practical level and the theoretical level, when the underlying microstructure of the medium is not periodic, not to say random. The relation to domain decomposition type methods will be emphasized. The talk is based upon a series of joint and ongoing works with X. Blanc (Université Paris-Diderot) and P.-L. Lions (Collège de France), F. Legoll (Ecole des Ponts & Inria), A. Lozinski (Université de Besançon), U. Hetmaniuk (University of Washington in Seattle) and various other collaborators:


10:00-10:30 Poster Blitz IIC 2001

10:30-11:00 Coffee Break
Preconditioned Iterative techniques for geophysical electromagnetic problems

Hisham bin Zubair Syed  S. MacLachlan*

One of the ways to map the different conductive layers in Earth's crust is to construct a so-called forward model in terms of Maxwell's equations in the frequency domain. A popular decomposition approach is to consider the vector potential and solenoidal parts of the electrical field individually in the form of a coupled model. Suitable FEM discretization leads to a complex-valued block-structured matrix system for these two components; consequently, their equivalent real form is a 4x4 block structured system, half of which has a non-trivial nullspace due to the underlying curl-curl operator. In this talk, we present a block-structured preconditioner based on the Auxiliary-space Maxwell Solver (AMS; Hiptmair-Xu) approach for the curl-curl blocks, augmented with appropriate treatment for the significant off-diagonal blocks in the coupled system.

Some Simple Preconditioners for Unfitted Nitsche discretizations of high contrast interface elliptic problems

Blanca Ayuso de Dios*  K. Dunn  M. Sarkis  S. Scacchi

We present some basic preconditioning techniques for the solution of the linear systems arising from CutFEM and unfitted Nitsche finite element approximations to elliptic interface problems with discontinuous coefficients. We introduce simple one level and two level methods in the spirit of classical Schwarz and Dirichlet-Neuman (domain decomposition) methods. We analyse the asymptotic convergence of the proposed solvers, addressing their optimality and their robustness with respect to the coefficients and the interface-mesh configuration. We present extensive numerical experiments to verify the theory and assess the performance of the proposed preconditioners.

Solvers for CutFEM Interface Stokes Problems

Kyle G. Dunn*  Blanca A. de Dios  Marcus Sarkis  Simone Scacchi

In this talk we consider a class of Stokes interface problems which arise when an elastic membrane interacts with an incompressible fluid. We first develop a cut finite element method (CutFEM) based on Nitsche’s formulation and DG techniques when the membrane does not align with the finite element mesh of the fluid. Then we introduce and analyze robust domain decomposition preconditioners and present numerical experiments confirming the optimality of the proposed preconditioners with respect to mesh and interface parameters.

Domain decomposition preconditioner for mixed-dimensional flow problems in fractured porous media

Ana Budisa*  Eirik Keilegavlen  Jan Martin Nordbotten  Florin Adrian Radu
We are interested in the mixed-dimensional approach to modelling fractured porous media, where fractures and their intersections are represented as lower-dimensional structures and the mortar method is used for flow coupling between the matrix and fractures. The advantages of the model are immediate in handling complex geometries and large aspect ratios. However, the model has set new numerical challenges and developing a robust linear solver is still necessary. Our goal is to efficiently solve the single-phase flow problem by integrating into the numerical methods the critical role that fractures play in the system behaviour - global exchange of information through fracture flow. We exploit the natural domain decomposition setting imposed by the fracture networks, where fracture are taken as interfaces between subdomains. This approach provides a solver that combines the useful features of the model, such as high performance in case of fracture-dominant flow, but also shows robustness with regards to the system parameters (e.g. permeability, fracture aperture). The convergence and stability of the method is verified on several examples of fracture network configurations, and notable results in reduction of condition and iteration numbers are obtained for both cases of high and low fracture permeability.
On an efficient parallel implementation of adaptive FETI-DP

Axel Klawonn  Martin Kühn*  Oliver Rheinbach

Domain decomposition methods such as FETI-DP (Finite Element Tearing and Interconnecting - Dual Primal) and BDDC (Balancing Domain Decomposition by Constraints) are highly scalable parallel solvers for the numerical solution of partial differential equations (PDEs). However, the convergence behavior of FETI-DP and BDDC methods with a standard coarse space highly depends on the parameters of the underlying PDE. The convergence rate of both methods can deteriorate significantly if composite materials are considered. In such cases, problem-dependent (or adaptive) coarse spaces offer a remedy. In adaptive methods, difficulties arisen from highly heterogeneous materials are detected automatically and an adaptive coarse space is set up. These methods are thus characterized by great robustness. Though, for an efficient parallel implementation, different issues have to be tackled to reduce the computational overhead in the set up phase. We will present details of the set up of the adaptive method to implement the coarse space enrichment efficiently in a parallel context. We will present weak and strong scaling results to show the good parallel scalability of our method.

Certified convergence rate for GenEO-2 method with approximate coarse solve

Frédéric Nataf

Convergence of domain decomposition methods rely heavily on the efficiency of the coarse space used in the second level. The GenEO coarse space has been shown to lead to a fully robust two-level Schwarz preconditioner which scales well over multiple cores. The robustness is due to its good approximation properties for problems with highly heterogeneous material parameters. It is available in the finite element packages FreeFem++, Feel++ and recently in Dune and is implemented as a standalone library in HPDDM. But the coarse component of the preconditioner can ultimately become a bottleneck if the number of subdomains is very large and exact solves are used. It is therefore interesting to consider the effect of approximate coarse solves. We present theoretical bounds of the robustness of GenEO methods with respect to approximate coarse solves. Interestingly, the GenEO-2 method has to be modified in order to be able to prove its robustness in this context.

Robust Conforming Discretizations based on Adaptive BDDC and LOD-VMS and ACMS

Marcus Sarkis*  Alexandre Madureira

We consider finite element methods of multiscale type to approximate solutions of symmetric elliptic partial differential equations with heterogeneous coefficients without assuming regularity of the solution. The goal is to obtain a finite element method with $O(H)$–a priori error estimates in the energy norm with hidden constants independently of the coefficients and the coarse mesh parameter $H$. The methods are of Galerkin type and follows the Variational Multiscale–VMS and Localized Orthogonal Decomposition–LOD and Approximate Component Mode Synthesis–ACMS approaches in the sense that they decouple
global spaces into multiscale and fine subspaces. The multiscale basis functions are based on globalizing a class of deluxe adaptive coarse spaces encountered on Balancing Domain Decomposition by Constraints–BDDC type of preconditioners so that they have minimum global energy. We show that these multiscale basis functions decay exponentially fast independently of coefficient contrasts and therefore they can be localized.

Comparison of the GenEO coarse space and multipreconditioned iterations

Nicole Spillane

For problems with heterogeneous coefficients it has been shown that coarse spaces based on solving generalized eigenvalue problems and multipreconditioning provide two ways to speed up convergence. In this talk I will compare the behaviour of both methods on some test problems and investigate the pros and cons of each.

Chair: Daniel Szyld

A Domain Decomposed Learning Algorithm for Image Recognition

Xiao-Chuan Cai

Principal component analysis is one of the popularly used techniques for unsupervised learning, and it has many applications such as model order reduction for PDE related calculations, face recognition in image sciences etc. The method is relatively easy to implement, but because it involves the solution of a dense eigenvalue, or singular value, problem, the cost is high and the parallelization is quite difficult. In this talk, we discuss a multilevel domain decomposition approach and the method has much lower parallel complexity and it has reasonable accuracy for certain class of problems. This is a joint work with Jingwei Li.

Virtual coarse spaces for irregular subdomain decompositions

Juan G. Calvo

The construction of coarse spaces for irregular decompositions (as the ones obtained from mesh partitioners) usually involves functions that are discrete harmonic in the interior of the subdomains. Nevertheless, the Virtual Element Method provides a natural way to define virtual coarse functions for such irregular subdomains, and it is possible then to construct an extension operator $R_0^T$ that does require discrete harmonic extensions. We will discuss a study for nodal elliptic problems in two dimensions. In particular, when using a two-level overlapping Schwarz algorithm, the theoretical bound for the condition number of the preconditioned system is the same as in previous studies done by O. Widlund and C. Dorhmann. This extension operator saves computational time and it is suitable for general polygonal meshes and irregular subdomains. Numerical experiments that verify the result will be shown, including some with regular and irregular polygonal elements and with subdomains obtained by a mesh partitioner.
A Memory Efficient BDDC Algorithm for Higher Order Elements

Clark R. Dohrmann

In this talk, we present a memory efficient BDDC algorithm for higher order elements. The overarching goal of this work is to develop a preconditioner that can be used together with a matrix-free approach. In order to accomplish this goal, inexact subdomain solvers are used at the element level which avoid the need for large dense factorizations. Results for both tensor product and simplicial elements are discussed.

BDDC with adaptive coarse spaces for incompressible Stokes with continuous pressure

Stefano Zampini

In recent years, adaptive coarse spaces have received considerable attention from different research groups. In this talk we will present numerical results obtained extending the previously developed techniques for symmetric definite problems to symmetric indefinite problems. An application to the incompressible Stokes problem discretized with continuous pressure will be provided.

Chair: Rob Falgout

11:00-1:00

MS10:Parallel-in-time methods for highly concurrent architectures

A Space-Time Multigrid Method for Electrophysiology

Pietro Benedusi*, Patrick Zulian, Rolf Krause

We present a parallel and efficient multilevel solution strategy for solving a non-linear computational problem arising from electrophysiology: the electrical activation in the human heart. In particular, we solve with a semi-geometric multigrid method the monodomain equation discretised with space-time finite elements. While we use continuous finite elements in space, for stability reasons we adopt discontinuous elements in time. The monodomain equation is a non linear diffusion-reaction equation and it becomes hard to solve when realistic parameters are chosen. For the construction of coarse spaces in the spatial domain we use L2-projections. This approach allows representing the coarse levels of the multigrid hierarchy independently from the fine level mesh. Hence the simulation can be performed on arbitrary geometries in any dimension. We investigate how different block smoothers, coarsening strategies and ordering of the space-time variables effect the overall convergence and robustness of the solver. By means of numerical experiments we finally illustrate the scalability and the convergence of our multilevel solution strategy.

Parallelized space-time boundary element methods for the heat equation

Stefan Dohr*, Olaf Steinbach

The standard approach in space-time boundary element methods for discretizing boundary integral equations is using space-time tensor product spaces, originating from a separate decomposition of the boundary
∂Ω and the time interval (0, T). This space-time discretization technique allows us to parallelize the computation of the global solution of the whole space-time system. Instead of using tensor product spaces one can also consider an arbitrary decomposition of the whole space-time boundary Σ = ∂Ω × (0, T) into boundary elements. This approach additionally allows adaptive refinement in space and time simultaneously.

In this talk we consider the heat equation as a model problem and introduce a parallel solver for the space-time system. The space-time boundary mesh is decomposed into a given number of submeshes. Pairs of the submeshes represent blocks in the system matrix. Due to the structure of the matrix one has to design a suitable scheme for the distribution of the matrix blocks to the computational nodes in order to get an efficient method. In our case the distribution is based on a cyclic decomposition of complete graphs. We present numerical tests to evaluate the efficiency of the proposed parallelization approach.

The presented parallel solver is based on joint work with G. Of from TU Graz, J. Zapletal and M. Merta from the Technical University of Ostrava.

Preconditioners for a space–time finite element discretization of parabolic problems

Huidong Yang∗ Ulrich Langer

In this talk, we will present AMG and two-level BDDC preconditioners for a space–time finite element discretization of parabolic problems. The space–time finite element discretization is based on the recent work by U. Langer, S. Moore and M. Neumüller (2016), that was originally proposed in the space–time isogeometric analysis and considered time as another variable. In order to solve the arising linear system of algebraic equations, we need good preconditioners. In particular, we extend the conventional BDDC preconditioners mainly designed for the second–order elliptic boundary value problems to our space–time setting. Our numerical experiments show robustness of the proposed preconditioners.

Multigrid Reduction in Time for 1D Hyperbolic Problems

Alexander Howse∗ Hans de Sterck Rob Falgout Scott MacLachlan Jacob Schroder

The current trend in computer architectures is towards greater numbers of processors with little improvement in clock speeds, hence future computational speedups must be obtained through algorithms with greater concurrency. In such a situation sequential time stepping is a clear computational bottleneck due to the lack of parallelism in the time dimension. We consider the multigrid reduction in time (MGRIT) algorithm, an iterative procedure which uses multigrid reduction techniques and a multilevel hierarchy of coarse time grids to allow temporal parallelism. In this talk, we discuss recent results for MGRIT applied to 1D hyperbolic partial differential equations. In particular we consider the variable wave-speed linear advection equation and the inviscid Burgers’ equation. We investigate the effects of using spatial coarsening, spatial relaxations, or higher order space-time discretizations in the MGRIT framework. Serial and parallel numerical results illustrating these effects will be provided.
Domain Decomposition with Local Impedance Conditions for the Helmholtz Equation

Ivan G. Graham* Euan A. Spence Jun Zou

We analyse one-level additive Schwarz preconditioners for the Helmholtz equation (with increasing wavenumber $k$), discretized using fixed order nodal conforming finite elements on a family of simplicial fine meshes with diameter $h$, chosen to maintain accuracy as $k$ increases. The preconditioners combine independent local solves (with impedance boundary conditions) on overlapping subdomains of diameter $H$, and prolongation/restriction operators defined using a partition of unity. In numerical experiments we observe robust (i.e. $k$-independent) GMRES convergence, even when $H$ decreases to zero (as $k$ increases), provided the rate of decrease of $H$ is not too fast. This provides a highly parallel $k$-robust one-level domain decomposition method. We provide supporting theory for this observation by studying the preconditioner when applied to a range of absorptive problems, $k^2 \mapsto k^2 + i\varepsilon$, with absorption parameter $\varepsilon$, where $|\varepsilon| \lesssim k^2$, and including the “pure” Helmholtz case ($\varepsilon = 0$). Working in the Helmholtz “energy” inner product, we prove a robust (i.e. wavenumber-independent) upper bound on the norm of the preconditioned matrix, valid for all $\varepsilon$. Under additional conditions on $\varepsilon$, we also prove a strictly-positive lower bound on the distance of the field of values of the preconditioned matrix from the origin. Combining these results with previous results of [M.J. Gander, I.G. Graham and E.A. Spence, Numer. Math. 131(3), 567-614, 2015] we obtain theoretical justification for the observed robustness of the preconditioner for the pure Helmholtz problem.

(Multilevel) low-rank correction methods for highly indefinite linear systems

Yousef Saad* Yuanzhe Xi

This presentation will discuss two classes of preconditioning techniques that can handle highly indefinite linear systems such as those that originate from wave propagation phenomena. The first class of methods that will be presented comprises multilevel techniques that take advantage of the so-called Hierarchical Interface Decomposition, which are essentially algebraic versions of ‘wirebasket’ techniques used in classical Domain Decomposition (DD) methods. Within a DD framework, such decompositions lead to Schur complements whose inverses can be easily approximated from a recursively defined inverse of a certain matrix representing couplings at a certain level to which a low-rank correction is added. These methods have a number of appealing features. Because they are essentially approximate inverse techniques, they handle indefiniteness quite well. Furthermore, they are amenable to SIMD computations such those inherent to GPUs. The second method to be presented targets specifically very indefinite problems and exploits a similar divide-and-conquer approach. Here, by resorting to rational functions of $A$, the algorithm decomposes the spectrum of $A$ into two disjoint regions and approximates the restriction of $A^{-1}$ on these regions separately. We will show how these rational functions can be built so that they can be applied stably and inexpensively. An attraction of the proposed approach is that the construction and application of the preconditioner can exploit two levels of parallelism. In addition, the preconditioner can be modified at a negligible cost into a preconditioner for a near-by matrix of the form $A - cI$, which can be useful in some applications. The efficiency and robustness of the proposed preconditioner are demonstrated on a few tests with challenging model problems, including problems arising from the Helmholtz equation in three dimensions.
High Order Transmission Conditions for efficient and accurate DDM applied to the simulations of wave scattering

Matthieu Lecouvez*  Bruno Stupfel

The numerical computation of scattering problems by electrically large objects remains limited by computer resources, due to the large number of unknowns, especially when inhomogeneous materials are present. Such problems can be accurately solved by coupling a finite element (FE) method with an exact radiation condition prescribed on the outer boundary of the computational domain. Domain decomposition methods (DDM) are particularly attractive both for solving this coupling and for reducing the numerical cost of the FE part. The FE part is decomposed into several coupled subproblems which can be solved independently with efficient transmission conditions, thus reducing considerably the memory storage requirements. The global problem is then solved using a preconditioned GMRES. It is well known that the convergence rate of the GMRES strongly depends on the TCs, and some high order TCs (HOTCs) are proposed here for multilayer coated objects.

The first HOTCs we introduce are based on the exact impedance boundary conditions computed on an infinite planar coating. A spectral analysis shows evidence of their efficiency for solving the preconditioned DDM problem. However, they do not insure the well-posedness of the subproblems, unless sufficient conditions are applied to their coefficients, degrading their performances. Also, they make use of pseudodifferential operators and their implementation requires the use of additional unknowns on each interface, increasing the numerical cost of the method. This is why we propose a second set of simplified HOTCs that insure the well-posedness of each subproblem and reduce the number of iterations compared to optimized Robin-like TCs without increasing the computational cost. Finally, to enhance the efficiency of the solver, a compression algorithm is applied to the resolution of the integral representation, reducing drastically the memory requirement as well as the time of each matrix-vector product. Parallelization is achieved using MPI and threads, for both the solution of the subdomains and the integral representation, and we will present accurate numerical results obtained on the CEA supercomputer Tera 1000.

Optimized domain decomposition method with complete radiation boundary conditions

Seungil Kim*  Hui Zhang

We present an optimized nonoverlapping Schwarz method for solving the Helm-holtz equation in waveguides. A domain is decomposed into nonoverlapped layered subdomains along the axis of the waveguide and subdomain problems are supplemented with complete radiation boundary conditions for communicating data between neighboring subdomains. A CRBC is designed for high-order absorbing boundary conditions and interpreted as a rational function approximation to the Dirichlet-to-Neumann operator, whose coefficients can be selected in an optimal way so that it can minimize reflection coefficients and enhance the convergence of the nonoverlapping Schwarz method. We use the CRBC as transmission conditions for parallel optimized Schwarz method without overlap and double sweep Schwarz method. These algorithms can be employed efficiently for a preconditioner in GMRES implementations. Finally, numerical examples illustrating the superior performance will be presented.

Chair: Alison Malcolm

11:00-1:00  MS19: Industry Minisymposium  Arts-1049
The Convergence of Big Data and Extreme Computing

D. Keyes

Motivations abound for the convergence of large-scale simulation and big data: (1) scientific and engineering advances, (2) computational and data storage efficiency, (3) economy of data center operations, and (4) the development of a competitive workforce.

To take advantage of advances in analytics and learning, large-scale simulations should evolve to incorporate these technologies in-situ, rather than as forms of post-processing. This potentially reduces burdens of file transfer and the runtime IO that produces the files. In some applications, IO consumes more resources than the computation, itself. Smart steering may obviate significant computation, along with the IO that would accompany it, in unfruitful regions of physical parameter space, as guided by the in-situ analytics. In-situ machine learning offers smart data compression, which complements analytics in leading to reduced IO and reduced storage. Machine learning has the potential to improve the simulation, itself, since many simulations incorporate empirical relationships, such as constitutive parameters or functions that are not derived from first principles, but tuned from dimensional analysis, intuition, observation, or other simulations. Machine learning in-the-loop may ultimately be more effective than the tuning of human experts.

Flipping the perspective, simulation potentially provides significant benefits in return to analytics and learning workflows. Theory-guided data science is an emerging paradigm that aims to improve the effectiveness of data science models, by requiring consistency with known scientific principles (e.g., conservation laws). It is analogous to “regularization” in optimization, wherein non-unique candidates are penalized by some physically plausible constraint (such as minimizing energy) to narrow the field. In analytics, among statistically equally plausible outcomes, the field could be narrowed to those that satisfy physical constraints, as checked by simulations. Simulation can also provide training data for machine learning, complementing data that is available from experimentation and observation. There are also beneficial interactions between the two types of workflows within big data. Analytics can provide to machine learning feature vectors for training. Machine learning, in turn, can impute missing data and provide detection and classification. The scientific opportunities are potentially enormous enough to overcome the inertia of the specialized communities that have gathered around each of paradigms and spur convergence.

Optimization of Finite-difference Kernels on Multicore Architectures for Seismic Applications

K. Akbudak V. ´Etienne D. Keyes* S. Kortas H. Ltaief T. Malas P. Thierry T. Tonellot

The time-domain finite-difference method (TD-FDM) has been used in geophysics for decades for seismic modeling and imaging. It is the main workhorse for applications that require accurate solutions of the wave equation such as reverse time migration (RTM) or full waveform inversion (FWI). In this presentation, we investigate how spatial and temporal cache blocking techniques can speed up TD-FDM on multi-core architectures. We conduct our analysis on Shaheen, the supercomputer at the King Abdullah University of Science and Technology (KAUST). We present the achievable performances by using a Cache Aware Roofline Model (CARM). We discuss the implementations and the benefits of spatial and temporal cache blocking techniques individually, and we provide results that pave the way for achieving the maximum efficiency of TD-FDM.

Recent advances in Full Wave-Form inversion in seismic depth imaging

Henri Calandra
Seismic methods are based on the study of elastic waves propagating inside the earth. The main objective of Seismic depth imaging is to extract information describing the geological structure of the subsurface from the recorded data. Seismic depth imaging can be defined as an inverse problem with the main objective of finding the best model of the subsurface explaining the recorded data. Thanks to the fantastic progress of modern HPC it is now possible to formulate the inverse problem in seismic as an iterative optimization problem minimizing an objective function describing the distance between the observed and predicted data. This process is known as Full Wave-form Inverse problem (FWI). Each step of the iterative algorithm essentially consists of a forward propagation of the actual sources in the current model and a forward propagation (backward in time) of the data residuals. The correlation at each point of the space of the two fields thus obtained yields the corrections of the model parameters. In this talk, we will present the recent advances in full waveform inversion and discuss about the way forward. After an introduction to the Seismic depth imaging in O and G industry, we will introduce the full wave-form inverse problem principles and some examples showing the value of the FWI in the context of seismic depth imaging. We will then show how more advanced wave equation propagator closer to the physics improve the results of the FWI and finally we will discuss about some R and D directions addressing the current FWI limitations.

1:00-3:00 Industry Mixer and Poster Session IIC Atriums

Chair: Gabriele Ciaramella/Martin Gander

3:00-5:00 MS03:Domain-decomposition methods for integral equation problems

The reflection method, a method of boundary decomposition

Julien Salomon∗ Guillaume Legendre Philippe Laurent

The method of reflections was introduced by Smoluchowski in 1911 to study sedimentation phenomena. The idea was to calculate the velocity field of a fluid in a multi-particle domain by iteratively considering sub-problems with only one particle. In today’s applications, this method is often coupled with discretizations based on a representation of the field as a boundary integral. This leads to the solution of a system whose unknowns correspond to quantities located on the border of the domain. In this context, the method of reflections is tantamount to iterating on a decomposition of the domain boundary. In this talk, we interpret this method in terms of iterative corrections of subspaces for which we show the orthogonality of the projectors involved. This analysis is valid when all objects have the same type of boundary conditions and in this case leads to a proof of convergence. In the case of different objects, the projectors are not anymore orthogonal and an alternative analysis strategy provides sufficient convergence conditions.

Applications of the method of reflections to homogenization and sedimentation problems

Richard Höfer

In this talk I will consider the Poisson equation in a perforated domain. In this setting, I will explain how the parallel version of the method of reflections can naturally be formulated in terms of orthogonal projections. It will be shown how to use this method in order to analytically prove a classical homogenization result. Moreover, a similar method is used to derive macroscopic equations for inertialess particles in Stokes flows.
Numerical Implementation of the Reflection Method

Maxime Chupin

The method of reflection is an iterative procedure designed to solve linear boundary value problems set in multiply connected domains. Being based on a decomposition of the domain boundary, this method is well-suited to be coupled with discretization based on a representation of the field as a border integral such as boundary element method (BEM). This leads to the solution of a system whose unknowns correspond to quantities located on the edge of the domain. After a general presentation of the method, we will show how this method can be implemented in the context of BEM with some numerical results and how this method can be used for applications to the computation of the first order wave loads on offshore structures.

Two-level preconditioning for BEM with GenEO

Pierre Marchand

Domain Decomposition Methods (DDM), such as Additive Schwarz (AS), can be used to precondition linear systems arising from Boundary Integral Equations (BIE). Introduced in Hahne and Stephan (1996), this approach was widely studied since then and extended in various directions, see e.g. Heuer (1996) and Tran and Stephan (1996). The basic idea is to adapt the classical FEM-based AS (such as presented in Toselli and Widlund (2005)) to the BIE context: this includes a two-level preconditioner relying on a coarse space, which leads to theoretical bounds on the condition number.

Regarding the choice of relevant coarse spaces, important progress has been achieved in recent years for the FEM context. For the construction of coarse spaces, the Generalized Eigenproblems in the Overlaps (GenEO) has emerged as one of the most promising approaches for symmetric positive definite problems, see Spillane et al. (2014). Instead of solving a coarse problem on a coarse mesh, GenEO takes eigenvectors of well chosen local eigenproblems as a basis for the coarse space. As one of its interesting features, GenEO is only based on the knowledge of the stiffness matrix elements and discretization agnostic, left apart a few reasonable assumptions.

In this talk, we will present recent theoretical and numerical results in 2D and 3D aiming at adapting GenEO to the BIE context for symmetric positive definite problems on closed and open surfaces. Examples of applications are Laplace problems on screens or dissipative Helmholtz problems. This work is supported by the project NonlocalDD, research grant ANR-15-CE23-0017-01 from the French National Research Agency and the numerical results are obtained using HPC resources from GENCI- CINES (Grant 2017-A0020607330).

Chair: Xiao-Chuan Cai

Two-level overlapping Schwarz methods using constrained energy minimizing multiscale finite element functions

Hyea Hyun Kim* Eric Chung Junxian Wang

Two-level overlapping domain decomposition methods are considered for fast solvers for elliptic problems
with highly varying and random coefficients. The coarse problem in the two-level methods is obtained from constrained energy minimizing multiscale finite element functions. In the first step, a certain generalized eigenvalue problem is formed for each overlapping subdomain to select off-line basis functions, which correspond to problematic part of the solution. The off-line basis functions are then used to find coarse basis functions that will form the coarse problem of the two-level overlapping Schwarz methods. In more detail, the coarse basis functions are obtained by solving energy minimizing problems for each coarse block using the orthogonality to the off-line basis as constraints. The proposed method is shown to be less sensitive to the overlapping width of the subdomain partition as well as the coefficients, which is the main improvement over the previously developed methods. Numerical results are included.

Reduced Adaptive GDSW Coarse Spaces for the Two-Level Overlapping Schwarz Method

Alexander Heinlein  Axel Klawonn*  Jascha Knepper  Oliver Rheinbach  Olof Widlund

An adaptive coarse space for the two-level overlapping Schwarz method is presented that combines the ideas of adaptive GDSW coarse spaces with those of reduced dimension GDSW coarse spaces. Consequently, local eigenvalue problems are solved in order to construct additional coarse basis functions. In the present approach, the eigenvalue problems correspond to the vertices or ancestors, respectively, of the domain decomposition.

Isogeometric
Overlapping Schwarz methods for the Biharmonic equation

Luca F. Pavarino*  Durkbin Cho  Simone Scacchi

We construct and analyze a scalable overlapping Schwarz preconditioner for the biharmonic Dirichlet problem discretized with isogeometric analysis. This preconditioner is built by solving local biharmonic problems on overlapping subdomains that form a partition of the CAD domain of the problem and by solving an additional coarse biharmonic problem associated with the subdomain coarse mesh. An h-analysis of the preconditioner shows an optimal convergence rate bound that is scalable in the number of subdomains and is cubic in the ratio between subdomain and overlap sizes. Numerical results in 2D and 3D confirm this analysis and also investigate the good convergence properties of the preconditioner with respect to the isogeometric polynomial degree $p$ and regularity $k$.

A Three-Level Extension of the GDSW Overlapping Schwarz Preconditioner

Alexander Heinlein  Axel Klawonn  Oliver Rheinbach*  Friederike Röver

A three-level extension of the GDSW overlapping Schwarz preconditioner is presented, constructed by recursively applying the GDSW preconditioner to the coarse problem. Numerical results, obtained for a parallel implementation using the Trilinos software library, are presented for up to 90 000 cores of the JUQUEEN supercomputer. The superior weak parallel scalability of the three-level method is verified. For large problems and a large number of cores, the three-level method is faster by more than a factor of two, compared to the standard two-level method. The three-level method can also be expected to scale when the classical method will already be out-of-memory.
Towards a Scalable Parallel-in-Time Full Space Optimization Algorithm

Eric C. Cyr∗ Denis Ridzal

Transient PDE constrained optimization is challenging due to repeated forward and backward simulation. Using current approaches, when a simulation uses only a parallel spatial decomposition near the strong scaling limit, the time to solution for the optimization problem cannot be decreased by adding more computational resources. Addressing this issue requires algorithmic advancement in optimization algorithms and solution methods. This talk proposes a new parallel in time preconditioner for solving transient KKT systems arising in an inexact SQP algorithm. Our composite-step SQP algorithm utilizes inexact iterative solution of “benign” KKT systems, corresponding to a sequence of strictly convex quadratic programs. Its inexactness-handling mechanisms ensure global and fast local convergence. The preconditioner used to solve the KKT system is critical to the efficiency of this algorithm. Our preconditioner explicitly exposes continuity in time constraints using a time domain decomposition technique. These constraints are relaxed and the coupled forward-adjoint system is solved using a multigrid in time process. This talk will present the preconditioner and show results in prototypical scenarios indicating convergence independent of the number of time steps. The performance of the preconditioner is demonstrated to be independent of the number of time steps both when used to solve a standalone KKT system and when used within a Burgers equation constrained optimization problem.

Recent Advances with Multigrid Reduction in Time

Robert Falgout∗ Jacob Schroder

Since clock speeds are no longer increasing, time integration is becoming a sequential bottleneck. The multigrid reduction in time (MGRIT) algorithm is an approach for creating concurrency in the time dimension that can be exploited to overcome this bottleneck and is designed to build on existing codes and time integration techniques in a non-intrusive manner. In this talk, we will discuss recent progress in application areas such as power grid simulation and neural network training. We will also describe new features in our open source code XBraid, including a numerical optimization capability.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Analysis of Overlap in Optimized Waveform Relaxation Methods for RLCG Transmission Line Type Circuits

Pratik M. Kumbhar∗ Martin J. Gander

Among many applications of parallel computing, solving large systems of ordinary differential equations (ODEs) which arise from large scale electronic circuits, or discretizations of partial differential equations (PDEs), form an important part. A systematic approach for their parallel solution are Waveform Relaxation (WR) techniques, which were introduced in 1982 for circuit solver applications. These techniques are based
on partitioning large circuits into smaller sub-circuits, which are then solved separately over multiple time steps, and the overall solution is obtained by an iteration between the sub-circuits. However, this technique can lead to non-uniform and potentially slow convergence over large time windows. To overcome this issue, optimized waveform relaxation techniques were introduced, which are based on optimizing a parameter. We show how this method improves the convergence for RLCG transmission line type circuits. We introduce overlap between sub circuits and analyze its effect on the convergence factor. For R=0, we find that these RLCG circuit equations represent discretizations of the well known Maxwell equations. We relate these two models and give some asymptotic results.

Waveform Relaxation with Adaptive Pipelining

Benjamin Ong∗ Felix Kwok

The development of waveform relaxation methods has enjoyed recent activity due to its flexibility in the choice of spatial and temporal grids and integrators, and the capability for space-time parallelism, where multiple waveform iterates can be simultaneously computed in a pipeline fashion. In this work, we are interested in adaptively choosing the number of waveform iterates that are computed in a pipeline parallel fashion at each time step. We provide some numerical evidence that supports one’s intuition about the proposed Waveform Relaxation method with Adaptive Pipelining (WRAP), followed by an analysis of the convergence and # of iterations for the WRAP method applied to the homogeneous heat equation and a hyperbolic example.

Chair: Lesley James

3:00-5:00 M19:Industry Minisymposium Arts-1049

Upscaling From a MD Simulation to a Continuum Simulation: Hydraulic Fracture Behavior in Naturally Fractured Rock Masses.

Maurice B. Dusseault∗ Erfan Sarvaramini Robert Gracie

The development of a stimulated high permeability volume (SV) during hydraulic fracturing (HF) in a naturally fractured rock mass (NFR) is singularly challenging to simulate mathematically. Similar to the upscaling of molecular dynamics (MD) models, we seek to represent the behavior of a discrete array of interacting bodies by a continuum approximation in order to achieve a tractable simulation time, without introducing weak assumptions. The task is far more challenging than typical MD simulations because at the discrete level there are strong fabric issues (oriented joint sets, perhaps faults, and weak bedding planes), different and uncertain joint properties, Biot coupling, advective-conductive heat transfer, and flow in joint arrays with changing apertures. Complex discrete interaction laws for joints involve sliding Mohr-Coulomb friction with joint dilation (aperture increase), cohesion loss related to sliding and to extensional displacements across joints, strongly non-linear block contact stiffness behavior that deviates from Hertzian behavior, and loss of contacts during HF when some natural fractures become non-contacting. Furthermore, the rock blocks delineated by the joints in the SV possess anisotropic properties, and large-scale heterogeneity also exists.

We have developed a promising direction for upscaling. Our new upscaled HF model for SV simulation in a NFR is a typical Galerkin FEM approach, including full Biot coupling, but using a non-local plasticity...
formulation (with dilation) to track the evolution of bulk stiffness and fluid transmission properties. A key factor is to develop an upscaled constitutive law from a discrete element model (DEM – a version of MD), and we use the DEM method of UDEC\textsuperscript{TM} and 3DEC\textsuperscript{TM} to quantify relationships such as the upscaled stiffness changes as functions of average bulk strain. A representative elementary volume at a scale less than the upscaled model gives the constitutive mechanical law, and we use porosity change – the sum of the new aperture from extension and shear dilation – to govern the coupled changes in stiffness and flow properties in a non-linear relationship.

The preliminary results seem promising, and we have demonstrated a lack of mesh dependency (something that plagues conventional HF models in FEM formulations), rapid execution times, and results that look quite reasonable. 2-D and one 3D examples are given after the upscaling method is explained, and we also show that shut-in pressure analysis, a typical approach to evaluating a reservoir, make a great deal of sense. In terms of execution time, we compute in several minutes problems that took a week using commercial DEM software. Because the upscaled constitutive law is elasto-plastic (irreversible strains), the system retains memory of the fabric evolution. This approach can be incorporated into simulation programs for actual field use to aid in the design of HF processes involving NFRs where significant SVs are generated. It is sufficiently efficient to use in parametric analyses and Monte Carlo simulations.

**Numerical techniques for coupling different seismic wave simulations**

Longfei Gao

Wave simulation in earth media is substantial for seismic studies. The simulation configurations are often non-trivial and require special adaptations in numerical methods to achieve efficient simulations. We consider three scenarios where it is beneficial to combine wave simulations of different characteristics. First, we demonstrate how to combine finite difference simulations with different grid spacings to account for large variations in subterranean wave speeds. Second, we demonstrate how to combine finite element and finite difference simulations as an effective treatment to non-trivial topography. Finally, we demonstrate how to combine acoustic and elastic wave simulations in the finite difference framework for sub-salt imaging applications. In all three cases, the concept of discrete energy analysis is employed to derive the proper discretization operators and interface coupling procedures, leading to overall discretizations that preserve the energy-conserving property from the continuous wave equations.

**The present and future of seismic processing software for HPC**

Amik St-Cyr

Next to data sets from particle physics and astronomy, geoscience data sets are the largest and most complex ones in all of science and engineering: making most geoscientific applications data driven methods reliant on specialized HPC resources. It is conjectured that existing (physics based) and upcoming (deep learning enabled) subsurface imaging algorithms will only continue to consume the lion’s share of HPC resources in the O&G industry. The constant challenge of following the various trends in HPC architectures, and, quickly adapting large parts of our software portfolio to leverage any possible cost benefits, has lead us to adapt our development strategy. Finally, current efforts in our production seismic imaging software directed towards alleviating HPC software complexity as well as upcoming alliances with academia are discussed.
Convergence of classical and optimized Schwarz method for the 2-dimensional Maxwell’s equations with discontinuous coefficients and generalizations

Fabrizio Donzelli\textsuperscript{*} Alexander Bihlo Colin G. Farquharson Martin J. Gander Ronald D. Haynes

In this talk we consider the two dimensional Maxwell’s equations in the low-frequency and quasi-static approximation. The two dimensional Maxwell’s equations are derived from the full 3-dimensional Maxwell’s equations under the assumption that the three-dimensional geometry is translation invariant with respect to one dimension. They model the behaviour of electric and magnetic fields in the Earth subsurface. The measurement of such fields, which is conducted according to the magnetotelluric method, provides information about the spatial variation of the electrical conductivity in the Earth’s subsurface. If \(1/\nu\) is the electrical conductivity, which is typically a piece-wise constant positive function, \(\mu_0\) the magnetic permeability of free space, \(\omega\) is the angular frequency, the two dimensional Maxwell’s equations (in the TM mode) are derived to be \(\nabla \cdot (\nu \nabla u) - i\omega \mu_0 u = f\), with Dirichlet boundary conditions. The complex solution \(u\) represents the component of the magnetic field along a preferred direction. The problem is two dimensional since the geology of the subsurface is essentially invariant in a particular direction, the “strike” direction. In this talk, we present a class of domain decompositions for which the classical and the optimized zero-order Schwarz methods applied to the two-dimensional Maxwell’s equations are convergent. Next, we present similar results for a more general class of partial differential equations which include the two-dimensional Maxwell’s equation as a special case.

Local Fourier analysis of BDDC-like algorithms

Jed Brown Yunhui He\textsuperscript{*} Scott MacLachlan

Local Fourier analysis is a commonly used tool for the analysis of multigrid and other multilevel algorithms, providing both insight into observed convergence rates and predictive analysis of the performance of many algorithms. In this talk, we adapt local Fourier analysis to variants of two- and three-level BDDC algorithms, to better understand the eigenvalue distributions and condition number bounds on these preconditioned operators. This adaptation is based on a new choice of basis for the space of Fourier harmonics that greatly simplifies the application of local Fourier analysis in this setting. The local Fourier analysis is validated by considering the two dimensional Laplacian and predicting the condition numbers of the preconditioned operators with different sizes of subdomains. Several variants are analyzed, which can yield good improvements in performance for some, but not all, two- and three-level methods.

Asymptotic analysis for the coupling between subdomains in Discrete Fracture Matrix models

Martin J. Gander Julian Hennicker\textsuperscript{*}

Current Discrete Fracture Matrix (DFM) models, such as [Flauraud, E., Nataf, F., Faille, I., Masson, R., 2003, Domain Decomposition for an asymptotic geological fault modeling, Comptes Rendus à l’académie des Sciences, Mécanique, 331, 849-855], [Martin, V., Jaffré, J., Roberts, J. E., 2005, Modeling fractures
and barriers as interfaces for flow in porous media, SIAM J. Sci. Comput. 26 (5), 1667-1691], [Angot, P., Boyer, F., Hubert, F., 2009 Asymptotic and numerical modelling of flows in fractured porous media, ESAIM Mathematical Modelling and Numerical Analysis 23, 239-275], rely on ad hoc approximations in order to derive the matrix fracture coupling conditions. In our work, we present a derivation of the exact coupling conditions for DFM models based on Fourier analysis, and further obtain approximations of these coupling conditions, up to a certain order of a given quantity (fracture width, conductivity, resistivity), by truncating the corresponding asymptotic expansions. In a next step, we give estimates for the error of the so derived approximate models and compare them to existing models in the literature. Finally, we present some numerical tests, in order to assess the computational performance of the reduced models.

A guaranteed nonlinearly preconditioned inexact Newton algorithm based on domain decomposition method

Jizu Huang*

In the talk, we present a new nonlinearly preconditionner for inexact Newton algorithm based on the domain decomposition method. The inexact Newton algorithm is preconditioned by solving a subdomain minimization problem, which is derived from the original nonlinear system. Under some necessary assumptions, we prove that the inexact Newton algorithm with the proposed nonlinear preconditioner will stop after several iterations. Some numerical test cases are carried out to verify the efficiency of the presented nonlinear preconditioner, including the comparisons between the inexact Newton algorithm with the proposed preconditioner, and with other existing preconditioners, or without preconditioner.

5:00– Free Time
Discretizations based on BDDC/FETI-DP Techniques

Marcus Sarkis*  Alexandre Madureira

The goal is present finite element discretizations for second-order elliptic problems with heterogeneous and possibly with high-contrast coefficients. Based on adaptive BDDC/FETI-DP techniques and Variational Multiscale Methods–VMS and Localized Orthogonal Decomposition Methods, we design robust discretizations and establish robust and optimal a priori error energy estimates without assuming regularity on the solution.
Computation of High Frequency Waves in Unbounded Domains: Perfectly Matched Layer and Source Transfer

Zhiming Chen

The talk considers numerical techniques for solving high frequency time-harmonic waves in unbounded domains. We start by introducing the ideas of the radiation condition, the absorbing boundary condition and the method of perfectly matched layer (PML), which played important roles in solving scattering problems in unbounded domains. The focus will be a recently introduced source transfer domain decomposition method (STDDM) whose optimal complexity is proved in the case of constant wave number based on the convergence theory of PML method. Our numerical experiments show that STDDM can be used as an efficient preconditioner for solving scattering problems with heterogeneous wave numbers. The talk is based on joint works with Xueshuang Xiang.

A Two-Level Additive Schwarz Domain Decomposition Preconditioner for a Fourth Order Variational Inequality Using a Flat-Top Partition of Unity Method

Christopher B. Davis*  Susanne C. Brenner  Li-yeng Sung

In this talk, we investigate the use of a type of additive Schwarz preconditioner for a fourth order variational inequality. The problem is discretized by a flat-top partition of unity method and solved iteratively using a primal dual active set algorithm. The numerical algorithm will be presented and analyzed and numerical examples will be given to demonstrate the effectiveness of the method.

Strong convergence analysis of iterative solvers for random operator equations

Lukas Herrmann

For random operator equations, the classical theory of iterative solvers is not directly applicable, since condition numbers of system matrices may be close to degenerate due to non-uniform random input. As a main result, it is shown that iterative methods converge in the strong, i.e., $L^p$, sense if the random input satisfies certain integrability conditions. As a result, multigrid and domain decomposition methods are applicable in the case of elliptic partial differential equations with lognormal diffusion coefficients and converge strongly with deterministic bounds on the computational work which are essentially optimal. This enables the application of multilevel Monte Carlo methods with novel rigorous, deterministic bounds on the computational work, see L. Herrmann Strong convergence analysis of iterative solvers for random
FETI-DP for a DG Method for Multiscale Problems in High Contrast Media

Rui Du  Talal Rahman

In this paper, we consider the second order elliptic partial differential equations with highly varying (heterogeneous) coefficients on a two-dimensional region. The problems are discretized by a discontinuous Galerkin (DG) method with the admissible functions restricted to a conforming finite element (FE) space in each subdomain, the so-called composite FE-DG method. The fine grids are in general nonmatching across the subdomain boundaries. A FETI-DP preconditioner is proposed and analyzed to solve the resulting linear system. It is proved that the condition number of the preconditioned linear system only depends on the coefficient contrast in a boundary layer of width $h$ along the subdomain interface, and quadratically on $H/h$, where $H$ is the subdomain diameter and $h$ is the fine mesh size. The quadratic dependence on $H/h$ becomes $H/h(1 + \log H/h)$ under a stronger assumption on the coefficients in the interior of the subdomains. Numerical results are presented to support our theory.

FETI-DP for the Three Dimensional Virtual Element Method

Daniele Prada  Silvia Bertoluzza  Micol Pennacchio

We deal with the Finite Element Tearing and Interconnecting Dual Primal (FETI-DP) preconditioner for elliptic problems discretized by the virtual element method. We extend the result of (S. Bertoluzza, M. Pennacchio, D. Prada, BDDC and FETI-DP for the virtual element method, Calcolo 54 (2017), 1565–1593) to the three dimensional case. We prove polylogarithmic condition number bounds, independent of the number of subdomains, the mesh size, and jumps in the diffusion coefficients. Numerical experiments validate the theory.

A Geometry-aware Hybrid Finite Element and Boundary Integral Equation Domain Decomposition Method for Maxwell’s Equations

Zhen Peng  Shu Wang

Fast, scalable and robust solution of the hybrid finite element-boundary integral (FE-BI) linear system of equations is traditionally considered a challenge due to multi-faceted technical difficulties. This work proposes a novel geometry-aware domain decomposition (DD) preconditioning technique for iteratively solving hybrid FE-BI equation. The technique ingredients include a volume-based Schwarz FE DD method and a surface-based interior penalty BI DD method. Comparing to previous algorithms, the work has three major benefits: (i) it results in a robust and cost-effective preconditioning technique for the solution of the FE-BI linear system of equations; (ii) it provides a flexible and natural way to set up the mathematical
models, to create the problem geometries and to discretize the computational domain; (iii) it has the potential to be a suitable paradigm for the parallel implementation of FE-BI algorithms on massively parallel computing architectures. The capability and performance of the computational algorithms are illustrated and validated through numerical experiments.

Non overlapping domain decomposition methods with non local transmission conditions for electromagnetic wave propagation

Emile Parolin

In this work, we investigate new iterative non overlapping domain decomposition methods for the numerical solution of time harmonic Maxwell’s equations. The main novelty of our approach is the use of non-local operators (integral operators) in the transmission conditions between two adjacent subdomains, in order to ensure an exponential rate of convergence, in the spirit of previous works for the scalar Helmholtz equation. The main theoretical aspects of the method will be detailed and preliminary numerical results will be presented.

On the Numerical Analysis of the Many-Body Dielectric Problem in Electrostatics

Muhammad Hassan* Benjamin Stamm

We consider the problem of calculating the electrostatic interaction between dielectric spheres embedded in a polarisable continuum. In order to solve this problem, E. Lindgren et al. have proposed a numerical method based on a Galerkin discretisation of an integral equation formulation of this problem. The proposed method is general enough to treat any homogeneous dielectric medium containing an arbitrary number of spherical particles of any size, charge, dielectric constant and position in the three-dimensional space. Furthermore, numerical experiments indicate that the algorithmic complexity of the method scales linearly with respect to the number of particles thanks to the use of a modified Fast Multipole Method. The current talk will present some first results on the numerical analysis of this algorithm. We show that the underlying integral equation can be interpreted as a linear operator equation involving a bijective integral operator on suitable Hilbert spaces, so that the integral equation formulation is well-posed in the sense of existence and uniqueness of solutions. In addition, we demonstrate that the structure of the equations leads to a simple iterative scheme involving a contractive integral operator, and we explore the dependence of this contraction factor on physical parameters such as the dielectric constant of the spheres and the medium, and the minimal separation between individual spheres. Finally, we discuss the well-posedness of the Galerkin discretisation of this integral equation formulation.

Analysis of the parallel Schwarz method for growing chains of fixed-sized subdomains

Gabriele Ciaramella* Martin J. Gander

A new class of Schwarz methods was recently presented in the literature for the solution of solvation models, where the electrostatic energy contribution to the solvation energy can be computed by solving a system of elliptic partial differential equations. Numerical simulations have shown an unusual convergence behavior of Schwarz methods for the solution of this problem, where each atom corresponds to a subdomain: the convergence of the Schwarz methods is independent of the number of atoms, even though there is no coarse grid correction. Despite the successful implementation of Schwarz methods for this solvation model, a rigorous analysis for this unusual convergence behavior is required, since no theoretical results are given.
in the corresponding literature.
In this talk, we analyze the behavior of the Schwarz method for the solution of a chain of atoms and show that its convergence does not depend on the number of atoms (subdomains). We use two different techniques to prove this result. The first technique is based on a Fourier expansion of the error and the analysis of transfer matrices constructed for an approximate model. The second one consists in an application of the maximum-principle and allows us to analyze very general geometries.

Chair: Axel Klawonn

10:30-12:30 MS06:Extremely parallel domain decomposition methods and their applications

A Scalable Implicit Navier-Stokes Solver on Unstructured Grid on Many-Core Machine

Xiao-Chuan Cai* Rongliang Chen

In this talk, we present some preliminary studies of an implicit, unstructured grid, Navier-Stokes solver on the Sunway TaihuLight supercomputer, whose processors include management processing cores (MPCs) and computing processing cores (CPCs). Newton-Krylov-Schwarz (NKS) is the general framework that we use to solve the large sparse nonlinear system and an optimally scheduled, small block Gauss-Seidel/Jacobi algorithm is introduced as the subdomain solver of NKS on CPCs. The focus of the talk is the refactorization and communication avoiding parallelization of the solver. We report some performance results obtained using a large number of MPCs and CPCs. This is a joint work with Lilei Wu, Li Luo, Zhengzheng Yan, and Xiao-Chuan Cai.

FROSCh - A Parallel Implementation of the GDSW Domain Decomposition Preconditioner in Trilinos

Alexander Heinlein* Axel Klawonn Oliver Rheinbach

The FROSCh (Fast and Robust Overlapping Schwarz) library, a parallel implementation of the GDSW (Generalized Dryja Smith Widlund) preconditioner, has recently been integrated into Trilinos as part of the package ShyLU. The GDSW preconditioner has been introduced by Dohrmann, Klawonn, and Widlund in 2008 and is a two-level overlapping Schwarz preconditioner with an energy-minimizing coarse space that is inspired by non-overlapping domain decomposition methods, such as FETI-DP and BDDC methods. It is robust for a wide class of problems, e.g., solid or fluid mechanics, and can be constructed in an algebraic way. In particular, the coarse space can be constructed from the fully assembled matrix without an additional coarse triangulation, even for irregular subdomains. However, the preconditioner can benefit from additional information about the problem. This talk gives an overview of the FROSCh code, its features, and user-interface and shows the parallel scalability and robustness of the solver for several problems. In particular, FROSCh is applied to scalar elliptic problems, linear elasticity, and nonlinear elasticity in fluid-structure interaction applications and as a monolithic preconditioner for saddle-point problems. Parallel scalability of the code is shown up to a maximum of 64K cores using a direct coarse solver on one core.
Comparison of Various Extremely Parallel Inexact BDDC Approaches and their Application to Nonlinear Problems

Axel Klawonn  Martin Lanser*  Oliver Rheinbach

The numerical solution of nonlinear partial differential equations, e.g., nonlinear elasticity or elasto-plasticity problems, on modern and future supercomputers requires fast and highly scalable parallel solvers. Domain decomposition methods such as FETI-DP (Finite Element Tearing and Interconnecting - Dual Primal) and BDDC (Balancing Domain Decomposition by Constraints) are such robust and efficient methods, and they are widely used to solve problems arising in the field of structural mechanics, e.g., the simulation of elastic or plastic deformations. In this talk, we will present a highly efficient BDDC implementation, realized in PETSc, and provide a comparison between different inexact variants known from the literature. We will discuss the advantages and disadvantages of the different approaches and present them in a common notation for the first time. We present weak scaling results up to hundreds of thousands of parallel processes and study the parallel scalability of all methods. We apply the inexact BDDC preconditioners to nonlinear problems using Nonlinear-BDDC. In Nonlinear-BDDC, local nonlinear problems are solved on the interior part of each subdomain, which, in many cases, improves the convergence speed of Newton’s method. It can be observed that Nonlinear-BDDC often allows the application of larger loads in nonlinear elasticity or elasto-plasticity problems. We also present a new approach, NL-ane-BDDC, which is a variant of Nonlinear-BDDC. Here, controlling the global energy of the given problem helps to increase the robustness of Nonlinear-BDDC.

Power and Energy Efficiency of Nonlinear Domain Decomposition Methods

Axel Klawonn*  Martin Lanser  Oliver Rheinbach  Matthias Uran  Gerhard Wellein  Markus Wittman

Nonlinear domain decomposition (DD) approaches are solution methods for nonlinear finite element problems based on a domain decomposition of the nonlinear problem. In recent years, many nonlinear DD approaches have been introduced and their superiority over the classical combination of a nonlinear solver, e.g., Newton’s method, with a linear DD approach has been shown for many model problems. Nevertheless, in nonlinear DD methods, many decoupled local nonlinear problems have to be solved in parallel, which can lead to a certain load imbalance. We propose to use a non-blocking MPI Barrier and to set idle cores to sleep, in order to save energy. It can be shown that nonlinear DD methods can save a significant amount of energy compared to classical approaches and even a better power efficiency can be obtained.

Optimized transmission conditions for discrete diffusion problems

Laurence Halpern*

We present discrete optimized Schwarz methods for anisotropic diffusion problems. We derive convergence factors to determine the optimal choice of parameters in the transmission conditions, and we study the best approximation problem in finite domains. We show that the performance of the algorithm can be greatly
improved, replacing the optimal parameter coming from the continuous analysis by a discretely optimized parameter for the bounded domain. We present a detailed numerical analysis as well and explain carefully the behavior of the algorithm, both in the overlapping or nonoverlapping case, for Robin and Ventcell Schwarz algorithms. This is a joint work with Martin Gander (Université Genève, Switzerland), Florence Hubert (Université Marseille, France), Stella Krell (Université Nice, France)

Optimized Schwarz-based nonlinear preconditioning for elliptic PDEs

Felix Kwok* Yaguang Gu

One way to accelerate the numerical solution of a nonlinear elliptic problem is to use nonlinear preconditioning, which replaces the original discretized problem by an equivalent but easier one. A well-known domain decomposition-based nonlinear preconditioner is the Additive Schwarz Preconditioned Inexact Newton (ASPIN) method, which was introduced by Cai and Keyes (2002). More recently, Dolean et al. (2016) derived the Restricted Additive Schwarz Preconditioned Exact Newton (RASPEN) method by considering the fixed point form of the nonlinear Restricted Additive Schwarz method, and showed that it compares favourably with existing methods. In this talk, we will study the behaviour and performance of a version of RASPEN that uses optimized transmission conditions. In particular, we show how a good choice of Robin parameters leads to significant reduction in the number of GMRES iterations required by the outer Newton loop. We show as examples an overlapping method applied to a heterogeneous problem, as well as a non-overlapping method for the Richards equation.

Optimized Schwarz methods for multiscale elliptic PDEs

Sébastien Loisel* Hieu Nguyen Robert Scheichl

The finite element method is widely used to approximate the solution of boundary value problems. This results in high-dimensional linear problems that are typically solved iteratively, e.g. using GMRES. If GMRES is to converge quickly, one needs a good preconditioner. The Schwarz method is a domain decomposition preconditioner that is well suited for parallel computation on supercomputers. Where the Schwarz method uses Dirichlet boundary conditions along the artificial interfaces, the optimized Schwarz method uses Robin boundary conditions. By choosing the Robin parameter carefully, one obtains faster convergence of the iterative scheme. When the underlying boundary value problem is heterogeneous, the performance of various domain decomposition preconditioners deteriorate. For example, when a fluid flows through a porous medium, certain flows may occur on a very rapid time scale and require very little energy. One way of accelerating domain decomposition algorithms for heterogeneous problems is to incorporate such low-energy features into the coarse space of the method. For a classical Laplacian on a rectangle, low-energy modes coincide with low frequency sine waves, but for heterogeneous problems, low-energy modes can take on a much more complex character. One way of automatically detecting these low energy modes is by solving small eigenproblems on each subdomain. The low energy eigenvectors can then be stitched together to obtain solutions whose energies are globally low. In this talk, we will show how such “spectral coarse functions” can be incorporated into the coarse space of an optimized Schwarz method. We will provide an analysis and numerical experiments that show that our analysis is sharp.
The Domain Decomposition Method of Bank and Jimack as an Optimized Schwarz method

Parisa Mamooler∗ Martin J. Gander Gabriele Ciaramella

In 2001, Bank and Jimack introduced a new domain decomposition algorithm for the adaptive finite element solution of elliptic partial differential equations. The novel feature of this algorithm is that the subdomain problems are defined over the entire domain, consisting of a fine grid in the area where the subdomain is responsible for an accurate solution, and a coarse grid elsewhere. A convergence analysis of this algorithm was given in 2008 by Bank and Vassilevski. We are interested here in understanding what the precise contribution of the outer coarse mesh is to the convergence behavior of the domain decomposition method proposed by Bank and Jimack. We show for a two subdomain decomposition that the outer coarse mesh can be interpreted as computing an approximation to the optimal transmission condition represented by the Dirichlet to Neumann map, and thus the method of Bank and Jimack can be viewed as an optimized Schwarz method, i.e. a Schwarz method that uses Robin or higher order transmission conditions instead of the classical Dirichlet ones. In particular, we show that when applied to the Laplace equation in one spatial dimension, the algorithm of Bank and Jimack computes an optimal Robin parameter for any choice of the outer coarse mesh, and the method thus converges in two iterations in this case. We then present more general situations, and we illustrate our results with numerical experiments.

Chair: David Moulton
10:30-12:30 Contributed Talks Arts-2071

Theory and collocation solvers for integral-algebraic equations

Hui Liang∗ Hermann Brunner

‘Mixed’ systems of integral-algebraic equations (IAEs) consisting of second- and first-kind Volterra integral equations (VIEs) arise in many mathematical modelling processes; we mention memory kernel identification problems in heat conduction and viscoelasticity, evolution of a chemical reaction within a small cell, and Kirchhoffs laws. In this talk, first, we will give some applications and motivations for IAEs. Second, the tractability index is introduced based on the $\nu$-smoothing property of a Volterra integral operator for general systems of linear IAEs, and the given IAE system is decoupled into the inherent system of regular second-kind VIEs and a system of first-kind VIEs. Next, the collocation solvers are applied to the decoupled index-1 IAE, and the optimal convergence properties of piecewise polynomial collocation solutions are derived. At last, we will give a counter-example to show that not all collocation solvers are feasible for index-2 IAEs, or for higher-index IAEs, and some other bottlenecks and unsolved problems will also be identified, which indicate that other efficient and faster solvers, including a possible application of domain decomposition (DD) methods, are needed. And we will also list some of our ongoing work.
A nonlinearly preconditioned inexact Newton method for blood flow problems in patient-specific arteries with stenosis

Li Luo∗ Wen-Shin Shiu Rongliang Chen Xiao-Chuan Cai

Simulation of blood flows is a promising tool for understanding the sophisticated hemodynamics in the arteries, especially for the situation of stenosis. In this talk, we present a numerical study for the blood flow in patient-specific arteries based on an unsteady model combining the incompressible Navier-Stokes equations with the resistive boundary condition. The governing equations are discretized by a stabilized Galerkin finite element method in space and a fully implicit second-order backward scheme in time. The resulting nonlinear system at each time step is solved by using an inexact Newton method with a domain decomposition based linear solver for parallelization. To improve the convergence and robustness of the Newton method, we develop an adaptive physics-based nonlinear elimination preconditioner which performs subspace correction to remove the local high nonlinearities. Numerical experiments are presented to demonstrate the superiority of the proposed algorithm over the classical method with respect to some physical and numerical parameters. We also report the parallel scalability of the proposed algorithm on a supercomputer with thousands of processors.

A hybrid transport-diffusion method for laser fusion simulation

Shuanggui Li∗ Xudeng Hang JingHong Li

Radiation plays a very important role in the transfer of energy in the indirect manner of Inertial Confinement Fusion (ICF). The photons, emitted by the ICF hohlraum wall after absorbing the incident laser energy, constitute the radiation field and ablate the capsule at the hohlraum center, and then drive implosion. These problems require accurately simulation not only fluid motion (including shock propagation) but also the transport of radiation energy density in both optically thick and thin materials in as computationally expedient a method as possible. For ICF experimental hohlraum we use domain decomposition method for integral simulation, while radiation transport equation is solved in the low-Z material region, and radiation diffusion equation is solved in the high-Z material region. Operator splitting method is applied for solving the strong coupled radiation hydro-dynamics system. The coupling conditions at the material interface are also discussed. Last, we give some numerical results to show the accuracy and efficiency of our hybrid method.

Schwarz methods for the implicit closest point method

Ian May∗ Ronald D. Haynes Steven Ruuth

The numerical treatment surface intrinsic elliptic PDE presents several interesting challenges not present in at space. The discretization of such PDE generally proceeds by either parameterizing the surface or embedding it into a higher dimensional at space. The Implicit Closest Point Method, (ICPM) is such an embedding method well suited to these problems, and allows the treatment of fairly general surfaces, \( S \), by requiring only minimal information about the surface itself. At the core of the ICPM lies an extension operator bringing surface bound information into the embedding space by enforcing constancy along the surface normals. With this extension operator the surface PDE can then be solved by standard methods on the embedding space, usually requiring a discretization only over a tubular neighbourhood of the surface. As a model equation, the positive Helmholtz equation, \((c - \Delta_S)u = f\), is considered. ICPM discretization considered here uses tensor product barycentric Lagrange interpolation to define the extension operator and

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standard second order centered differences for the ambient Laplacian. Under this scheme a non-symmetric system with some complex eigenvalues is obtained. Furthermore, the extension operator introduces some weak non-locality, and depending on the degree of polynomials, a system with poor sparsity. These properties reduce the utility of iterative solvers and motivate the development of strong preconditioners. Optimized restricted additive Schwarz (ORAS) methods are well suited to this task and are formulated herein. The interesting geometry of the problem presents challenges for the construction of sub-domains over the tubular mesh as well as the enforcement of Robin boundary operators, the resolution of which will likely be of use in other applications. Finally, the obtained solvers and pre-conditioners are compared with standard RAS and unpreconditioned GMRES, showing a reduction the required iterations in all tested problems.

Domain decomposition tips the scales: From additive Schwarz methods to homogenization theory and beyond

Daniel Peterseim*

Homogenization theory is a very powerful tool of mathematical modeling and analysis that serves as the theoretical backbone of many efficient numerical methods for multiscale partial differential equations (PDEs). This talk aims to show that, conversely, numerical techniques such as domain decomposition can be the basis for proving homogenization results on the PDE level. The starting point of this venture is the localized orthogonal decomposition approach to the numerical homogenization of second order linear elliptic PDEs with arbitrarily rough diffusion coefficients. The method is phrased in terms of a subspace decomposition into a coarse finite element space and local overlapping patch spaces. The associated discrete effective problem is reinterpreted by means of an integral operator acting on standard finite element spaces. The convergence theory of additive Schwarz methods proves the exponential decay of the involved integral kernel. This motivates the use of a diagonal approximation of the kernel which turns out to be the classical homogenization limit in the case of periodic coefficients. Another surprising application of such non-standard arguments is the quantified localization of eigenstates of linear Schrödinger operators under disorder potentials.

The main results of this talk are based on joint works with R. Kornhuber and H. Yserentant as well as D. Gallistl.

References:


Integration of fully 3D fluid dynamics and coastal circulation models

Hansong Tang*  Yingjie Liu  Wenbin Dong

Now there is need to simulate in high fidelity many multiscale and multiphysics coastal flow problems, such as oil spill from bottom of an ocean and impinging of storm surge onto a coastal bridge. In order to simulate such problems, especially those small-scale, complicated, local flows, a fully 3D fluid dynamics model and a coastal circulation model are integrated into a single modeling system. In particular, the full Navier-Stokes equations for the fully 3D fluid dynamics model and the geophysics fluid dynamics equations for the circulation model are coupled in two-way with each other. In this presentation, integration of a fully 3D fluid dynamics model that we developed for small-scale, local flows and an actual coastal ocean model widely used in the community for large-scale ocean currents is presented. Integration methods, transmission conditions, and interface algorithms are discussed, and numerical experiments are provided to demonstrate the performance of the proposed system and difficulties involved. Example applications to flow problems with realistic coastal settings will also be given to illustrate the system’s unique capability in capturing practical multiphysics phenomena at distinct scales.

A framework for seamless one-way domain nesting of internal wave-resolving ocean models

Justin Rogers*  Oliver Fringer  Dong Ko

Large scale ocean models are increasingly more resolved in space and time including recently resolving internal tidal motions. However, nested child grids with higher resolution are required to accurately simulate internal wave propagation, steepening, and flow interaction with bathymetry. In this framework, there lies a fundamental problem of information propagation, where the child grid computes a different solution than the parent grid at the outgoing boundary and thus the boundary condition is indeterminate. In addition, without damping, boundary conditions are typically reflective to wave energy. To solve this ambiguity within the SUNTANS model, we present a novel new approach to force hydrodynamic flows including internal wave motions from the parent grid to the child grid by splitting the velocity and forcing into four components of Barotropic low frequency (mean flows), Barotropic high frequency (tides), Baroclinic low frequency, and Baroclinic high frequency (internal waves) where low frequency is $O$(days) and high frequency is $O$(hours). The high frequency Baroclinic component of velocity is forced on the boundaries for energy flux into the domain, while the low frequency velocity and scalars are nudged to the parent grid over the entire domain. A sponge layer on the exterior damps all outgoing baroclinic wave motions but allows other flows to pass through. This method overcomes the inherent error associated with approximate radiative boundary conditions for outgoing internal wave energy. A series of idealized simulations demonstrate the functionality of this method, with a goal of nesting the SUNTANS nonhydrostatic model within the NCOM global model with resolved internal tides.
Domain Decomposition in Climate Models

Robert Jacob∗ Vijay Mahadevan Pavel Bochev

Numerical models of the climate system are one of the canonical multi-scale and multi-physics problems. Their domain is the entire planet and they typically decompose this domain into four major components representing the global atmosphere, ocean, land surface and sea ice. Additional domains added recently include river systems and ice sheets. Different equation sets must be solved in each domain and each domain often has its own numerical grid. The technical challenge of uniting these different systems in one program has been accomplished through libraries such as the Model Coupling Toolkit and a custom "coupler" driving the enter system. Traditionally an ad-hoc loose coupling strategy has been employed to integrate the different models together in time. The coupler exchanges appropriate information between the components, based on their states at the previous time interval and marches these components forward in time independently from each other. Only recently have the possible numerical instabilities and errors from these approaches been considered and alternatives explored. Despite the approximations, climate models have considerable skill in reproducing observed climate of the 20th century.

Toward improved ocean-atmosphere coupling algorithms

Eric Blayo∗ Florian Lemarié Charles Pelletier

The interactions between atmosphere and ocean play a major role in many geophysical phenomena, covering a wide range of temporal scales (e.g. diurnal cycle, tropical cyclones, global climate...). Therefore the numerical simulation of such phenomena require coupled atmospheric and oceanic models, which properly represent the behavior of the boundary layers encompassing the air-sea interface and their two-way interactions.

However deficiencies appear in current ocean-atmosphere coupled models, both in the formulation of the physical parameterizations and in the algorithmic approach used for the coupling. Parameterizations used for representing the oceanic and atmospheric boundary layers and for computing the air-sea fluxes are generally developed independently, without any guarantee regarding the well-posedness of the overall coupled problem. Moreover usual coupling algorithms exhibit synchrony issues.

In this talk, we address these problems from the point of view of domain decomposition methods. We show that present coupling methods used for ocean-atmosphere coupled models can be written in the formalism of Schwarz iterative algorithms, and correspond to methods that are not pushed to convergence, which may lead to quite imperfect coupling. We discuss the objective of achieving a mathematically and physically consistent ocean-atmosphere coupling, and we show that using improved coupling algorithms (like Schwarz methods) can impact the coupled model solution quite significantly.
From Capacitance Matrix Methods to Early Two-Level Iterative Substructuring Methods

Marcus Sarkis * Maksymilian Dryja

In this talk we revisit some of the developments made between the direct substructure methods introduced in the early '60s and the first international conference on domain decomposition methods, DD1, held in Paris in January 1987. Among these developments, we travel over Capacitance Matrix Methods, the seminal work by Proskurowski and Widlund in 1976 and some subsequent contributions that provided the initial basis for the area of iterative substructuring methods.

Algebraic view of Schwarz Methods

Daniel B. Szyld*

In this talk we review several results in which Schwarz methods are studied from an algebraic point of view, that is, when we consider matrices which may or may not come from discretizations of PDEs. Our first contribution using this algebraic view was to study the convergence of Restricted Additive Schwarz (RAS). Later on, we were able to study Optimized Schwarz methods (OSM). In particular these analyses can apply to matrices obtained from discretizing PDEs on irregular domains, or for graded meshes. Traditional analysis of OSM were restricted to the whole plane or half spheres.

BDDC for Weak Galerkin Discretizations

Xuemlin Tu* Bin Wang

The BDDC (balancing domain decomposition by constraints) methods have been applied successfully to solve the large sparse linear algebraic systems arising from conforming finite element discretizations of second order elliptic and Stokes problems. In this talk, the BDDC algorithm will be extended to the problems which are discretized using the weak Galerkin method, a newly developed nonconforming finite element method. The condition number bounds of the BDDC preconditioned operator are analyzed, and the same rate of convergence is obtained as for conforming finite element methods. Numerical experiments are conducted to verify the theoretical results.

Task-based Parallelization of Nonlinear Preconditioning

David Keyes*, Amani Alonazi, Lulu Liu, Li Luo

We present an asynchronous hybrid task-based implementation of nonlinearly preconditioned Newton iteration, applied to implicitly discretized systems of elliptically-dominated partial differential equations. Nonlinear preconditioning of a system of nonlinear algebraic equations tends to generate tasks of unequal
workload in different index-set partitions. For right-preconditioning based on sub-vector elimination, this is an intrinsic aspect of the method, and for left-preconditioning based on defining a new nonlinear residual vector, this is a consequence of the typical motivation for nonlinear preconditioning: different sub-problems have different degrees of “nonlinear stiffness”. Nonlinear preconditioning typically bets that global convergence can be obtained in relatively few synchronized global Newton iterations, within each of which perhaps many Newton iterations are performed on smaller local problems. In the typical bulk-synchronous setting of Newton solvers, many processors – potentially a vast majority – may sit idle awaiting the convergence of the more challenging subproblems.

The introduction of the Additive Schwarz Preconditioned Inexact Newton method (ASPIN, 2002) mentions that while ASPIN offers robustness and potentially improves overall arithmetic complexity, it may exacerbate issues of load imbalance. To prepare nonlinearly preconditioned solvers for systems in which bulk synchrony is impractical, including, for example, exascale systems of a billion cores, we explore and illustrate the performance of hybrid parallelization of nonlinear preconditioning using a dynamic runtime system that works off a directed acyclic dependency task graph.

Chair: Rob Falgout

3:15-5:15  MS10:Parallel-in-time methods for highly concurrent architectures  Arts-1045

The Performance of the PFASST Method on a Suite of Shallow Water Test Equations on the Rotating Sphere

Michael Minion*  Francois Hamon  Martin Schreiber

This talk will report on recent work to assess the parallel in time performance of the PFASST algorithm applied to a popular suite of test equations from the atmospheric modeling community. For this study, the PFASST algorithm is paired with a spatial discretization based on spherical harmonics and applied to popular test cases governed by the shallow water equations on a rotating sphere. The implementation uses the libpfasst library and the SWEET (Shallow Water Equation Environment for Tests) package. High-order semi-implicit or IMEX parallel in time schemes are tested with a careful consideration of the effects of viscosity and resolution on the parallel performance.

Parallel-in-time solution of the time-periodic eddy current problem with discontinuous excitation

Iryna Kulchytska-Ruchka*  Sebastian Schöps  Martin J. Gander  Innocent Niyonzima

In the present contribution we deal with mathematical models, which involve discontinuous right-hand sides. Such situations occur, e.g., in power engineering when electric devices are supplied with a pulse-width-modulated signal. In order to treat systems with such a quickly-switching (discontinuous) excitation we consider a modified Parareal method with reduced coarse dynamics. Its main idea is to solve the coarse problem with a low-frequency smooth input, which can be obtained, e.g., from Fourier analysis. Furthermore, during initial design stages of electromagnetic devices, when engineers only consider steady-state operating characteristics, solution of the time-periodic problem is particularly interesting. Adapting to the time-periodicity of the desired steady-state solution, we will apply the modified Parareal approach with reduced coarse dynamics to the time-periodic eddy current problem. Performance of the method is
illustrated via its application to the simulation of an induction machine.

Acknowledgement The work of I. Kulchytska-Ruchka is supported by the Excellence Initiative of the German Federal and State Governments, the Graduate School of Computational Engineering at TU Darmstadt, and the BMBF (grant No. 05M2018RDA) in the framework of project PASIROM.

Towards parallel in time methods for numerical weather prediction.

Jemma Shipton∗ Colin Cotter Beth Wingate Martin Schreiber

We present recent work on a parareal algorithm for solving the rotating shallow water equations on the sphere. The parareal algorithm has two ingredients: a cheap (coarse) integrator and a more accurate (fine) integrator. The efficiency of the scheme is determined by the rate at which convergence is achieved. It is therefore essential that the coarse integrator is sufficiently accurate to enable convergence, while remaining cheap enough that it is not a bottleneck that slows down the scheme. Our approach follows that of Haut, T. et al An asymptotic parallel-in-time method for highly oscillatory PDEs, 2014 which showed that averaging the nonlinear terms over fast oscillations includes the effects of near-resonances, essential for accuracy and hence convergence. A key component of this scheme is the computation of an approximation to the exponential of the linear operator corresponding to the fast linear waves in the system. Here we use a rational approximation [Haut, T. et al A high-order scheme for solving wave propagation problems via the direct construction of an approximate time-evolution operator, 2015]. This requires the solution of an elliptic problem for each term. The method is highly parallelisable but it is vital that the solution of each term is efficient.

In this talk, we will describe the construction of an efficient coarse integrator for the rotating shallow water equations and present the latest results from various test cases.

Understanding the effects of grid coarsening in space within the Parareal algorithm

Thibaut Lunet∗ Julien Bodart Serge Gratton Xavier Vasseu

Among all Parallel-in-Time solutions that are available today, Parareal has the great advantage of not requiring heavy implementation work to be used within any already existent time-stepping solver. In the particular case of an explicit solver, space coarsening can be used to define a coarse solver, that provides interesting properties in terms of accuracy and time-parallel speedup. However, a major drawback of Parareal is that numerical instabilities can be expected for advection dominated problems, if some simulation parameters are not chosen wisely, hence a loss of parallel speedup.

In this talk, we study the use of Parareal with space coarsening to solve the linear advection equation, by the mean of a Fourier analysis. The latter combines concepts from both Von Neuman analysis for space-time discretizations and Local Fourier Analysis for multi-grid methods. We identify the main effects of the grid coarsening on the convergence of Parareal, in order to bring some answers on the following questions:

• Can Parareal with space-coarsening be stable when used on the advection problem ?
• What is the influence of the chosen interpolation methods, and its order ?
• Does the initial solution play a role in the convergence of the parallel-in-time algorithm ?

Finally, a comparison to a bigger and more complex problem (Navier-Stokes equations) will be done to assess the generality of this analysis.
A Parallel Variational Mesh Quality Improvement Method

Suzanne Shontz* Maurin Lopez Weizhang Huang

There are numerous scientific applications which require large and complex meshes. Given the explosive growth in parallel computer architectures, ranging from supercomputers to hybrid CPU/GPU architectures, there has been a corresponding increase in interest in parallel computer simulations. For computational simulations involving the above applications, algorithms, which generate the mesh and manipulate it in parallel, are required. In particular, parallel mesh quality improvement is required whenever meshes of low quality arise in such simulations. In this talk, we describe our parallel variational mesh quality improvement method designed for distributed memory machines. The method is based on the sequential variational mesh quality improvement method of Huang and Kamenski. Although most mesh quality improvement methods directly minimize an objective function that explicitly specifies the mesh quality, Huang and Kamenski use the Moving Mesh PDE (MMPDE) method to discretize and find the minimum/maximum of a meshing functional, which is related to the mesh quality in an implicit manner. We solve the resulting ODE in parallel, which yields a mesh with a better quality. To solve the ODE in parallel, the mesh is first partitioned into regions using METIS. Next, the ODE is solved in parallel on the interior nodes of each mesh sub region. For nodes belonging to partition boundaries, i.e., those that are shared among cores, the algorithm calculates a partial ODE solution. To complete the solution at the shared nodes, a reduction operation using non-blocking MPI collective communication is performed. In order to overlap communication with computation, we experiment with various strategies for data organization. We test the performance of our method for up to 128 cores on tetrahedral meshes with up to 160M elements.

Using Massively Parallel Mesh Adaptation to Reach Large Scale Simulations on Tier0 supercomputers

Hugues Digonnet* Luisa Silva

Today, supercomputers have hundred of thousand cores, hundred of TB of memory and allow us to perform very large simulations (with meshes of up to several billion of nodes) if we are able to exploit their power. Exploiting such supercomputers needs the parallelization of the whole computing chain, from mesh generation to visualization. Here, we will present work performed to combine benefits from three main optimizations for FEM simulations: parallel computing, mesh adaptation and a multigrid solver. These three algorithmic optimizations allowed us to, respectively, increase the computational power (number of FLOPS/s) using a large amount of cores, reduce the problem size for a given error using heterogeneous mesh size (or a metricsfield), reduce the number of FLOPS needed for the resolution by reducing the algorithmic complexity to solve large linear systems. Taken individually, each of these optimizations already provides a nice improvement, but combining all of these make possible running really large scale simulations to obtain accurate results on complex data structure given by real world at Tier0 supercomputer scale.

In this paper, we will focus on anisotropic mesh adaptation optimization and present results obtained using full Tier0 supercomputers with around 100,000 cores. Two scalability tests have been considered: the first one consists in evaluating the parallelization strategy by building a large distributed mesh containing 1000 billion of elements in 2d and 3d; the second one considers heterogenous anisotropic meshes to well
Structured Meshes in a Task-based Parallel Framework

Navamita Ray*  Ben Bergen

Traditionally, multiphysics applications have followed a purely MPI-based or MPI+threads based distributed programming models targeted towards multicore systems. Upcoming heterogeneous architectures (such as Haswell and Knights Landing processing units in the next generation supercomputer like Trinity at Los Alamos National Laboratory (LANL)) provide greater concurrency through manycore layouts, as well as deep complex memory hierarchies, which necessitate the redesign of algorithms to take advantage of the high-degree of concurrency. Towards this end, research into various task-based runtimes have accelerated. In this talk, I will present the structured mesh topologies supported by a compile-time configurable multiphysics framework called FleCSI which provides control, execution, and data abstractions that are consistent with the state-of-the-art runtimes such as Legion, MPI, etc.

A surface moving mesh method based on equidistribution and alignment

Avary Kolasinski*  Weizhang Huang

We will introduce a new approach for variational mesh generation and adaptation on surfaces. We will then formulate a meshing functional for surface meshing that is based on the equidistribution and alignment conditions. Finally, we will present numerical results in both 2-D and 3-D.

Combining $h$- and $r$-adaptivity for finite-element models with jumping coefficients

Hormoz Jahandari*  Scott MacLachlan  Ronald D. Haynes

Discontinuous (jumping) coefficients often appear in modelling problems dealing with inhomogeneous media. An example of this is the geophysical electromagnetic (EM) problem, where these jumps occur at interfaces which separate regions of high conductivity contrasts. These interfaces, along with other problem features, such as singular EM sources and pointwise solution observations, motivate mesh refinement to achieve good accuracy. The goal of this study is to investigate the combined application of $h$- and $r$-refinement to reduce solution error in the modelling of EM data. We start in 1D to explore aspects of the $r$-adaptation before extending to higher dimensions. The steady-state diffusion and Helmholtz equations (which are commonly solved for the EM scalar and vector potentials, respectively) constitute the physical PDEs (PPDEs) here, while the $r$-refinement is based on an equidistribution principle. The PPDEs and the mesh PDEs are solved alternately in an iterative manner to reduce an error estimate to a desired level. At each iteration, the error estimate and its corresponding monitor function are updated and the mesh is $h$-refined accordingly. Various finite-element (FE) a posteriori error estimates and monitor functions were examined: while FE residual-based estimates were cheaper to compute, hierarchical error estimates were found to be better indicators of the true errors. Also, the equidistribution of the error-based monitor
functions was more efficient in reducing the error in comparison to a Hessian-based monitor function constructed from the hierarchical estimate.

A non-invasive implementation of mixed transmission conditions for a domain decomposition method - application to contact problems

Paul Oumaziz* Pierre Gosselet Karin Saavedra

In the last years, domain decompositions methods (DDM) have been adapted to tackle large nonlinear problems, but efficiency and robustness still remain a challenge. For nonlinearity “in the volume” relocalization approaches have proved their ability to cast the global problem into small independent nonlinear problems on the subdomains. For surface nonlinearity, frictional contact has also been inserted in the FETI framework and the Latin method which can also deal with cohesive interfaces. The Latin DDM can be viewed as a fixed point for which an iteration is decomposed into (i) a problem verifying only the relations of the interfaces and (ii) the subdomains’ equilibrium. Each step is linked to the other one through mixed transmission conditions. A non-invasive Latin DDM (i.e. without altering a FEM commercial software) has been proposed by the authors. Here, the mixed conditions were related to the stiffness of a new layer of elements patched on the subdomains’ boundaries. The optimal Robin parameters for the fastest convergence depends on global data which is too expensive in a parallel implementation. This work aims at proposing an automated choice of the Robin conditions for friction contact problems in the non-invasive framework. The idea is to approach the subdomains’ stiffness to adapt the one of the patched elements.

Domain Decomposition for the equations of linear elasticity in non homogenous materials

Kévin Santugini-Repiquet*

We consider the equations of linear elasticity, first for homogenous materials, then for heterogeneous materials. We consider both overlapping OSM (Optimized Schwarz method) and non overlapping OSM with various choices of transmission condition. We study the convergence of these methods when applied to linear elasticity problems. In particular, we study numerically how the speed of convergence varies depending on both the choice of transmission conditions between subdomains, and the width of the overlap.

Coupling Parareal and Dirichlet-Neumann/Neumann-Neumann Waveform Relaxation Methods for the Wave Equation

Bo Song* Yao-Lin Jiang

The Dirichlet-Neumann and Neumann-Neumann waveform relaxation methods are non-overlapping spatial domain decomposition methods to solve evolution problems, while the parareal algorithm is in time parallel fashion. Based on the combinations of space and time parallel strategies, we present and analyze parareal Dirichlet-Neumann and parareal Neumann-Neumann waveform relaxation for the wave equation. Between these two algorithms, parareal Neumann-Neumann waveform relaxation is a space-time parallel algorithm, which increases the parallelism both in space and time. We derive for the wave equation the convergence
results for both algorithms in one spatial dimension. We also illustrate our theoretical results with numerical experiments.

**Optimized Schwarz methods with elliptical domain decompositions**

Xin Chen  Martin J. Gander  Yingxiang Xu*

Differential models in elliptical geometries are critically important for problems such as water resource simulations, laser cutting and welding, and scattering problems. Optimized Schwarz methods are among the best parallel methods for such problems. Due to fast algorithms for Poisson equations in an elliptical geometry, it is critically important to decompose the computational domain into many elliptical rings when applying the optimized Schwarz methods, which is more efficient than decomposing the computational domain arbitrarily. However, optimized Schwarz methods with elliptical domain decomposition are still not well developed and a strategy using locally scaled optimized transmission parameters from straight interface analysis is generally applied in applications. In this talk, we show a rigorous analysis on a positive definite model problem for optimized Schwarz methods with elliptical domain decompositions and obtain many new results: first, we derive, based on careful analysis of a Mathieu-like equation, families of optimized transmission parameters and the corresponding asymptotic estimates for the convergence behavior in elliptical coordinates; second, we find that in Cartesian coordinates, the optimized transmission parameters are not constants any more along the interfaces, and hence, for example, a constant Robin parameter may not be the best choice, at least it is not close to the optimized transmission parameters we derived in the elliptical coordinates; and finally, we find that using the optimized parameters from the straight interface analysis scaled locally by the interface curvature is still effective in the asymptotic sense, although the performance deteriorates when the eccentricity of the interfaces goes to one. We use numerical examples to illustrate our analysis and findings.

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<td>Business Meeting for Scientific Committee Arts-2029</td>
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Thursday, July 26, 2018

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<td>8:30-9:15</td>
<td>Plenary Lecture-09 Xiaoye (Sherry) Li</td>
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<td>9:15-9:45</td>
<td>Plenary Lecture-10 André Fortin</td>
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Chair: Petter Bjørstad

8:30-9:15 Plenary Lecture-09 Xiaoye (Sherry) Li IIC-2001

Reducing flops, communication and synchronization in sparse factorizations

X. (Sherry) Li

Multiphysics and multiscale simulations often need to solve discretized sparse algebraic systems that are highly indefinite, nonsymmetric and extremely ill-conditioned. For such problems, factorization based algorithms are often at the core of the solvers toolchain. Apart from being used in direct solvers, they are also used as subdomain solvers in domain decomposition, coarse grid solvers in multigrid, and preconditioners in Krylov solvers, just to name a few.

Compared to pure iterative methods, the higher computation and communication costs in factorization methods present serious hurdles to utilizing extreme-scale hardware. I will present several research vignettes aimed at reducing those costs. By incorporating data-sparse low-rank structures, such as hierarchical matrix algebra, we can obtain lower arithmetic complexity as well as robust preconditioner. By replicating small amount of data in sparse factorization, we can avoid communication with provably lower communication complexity. By means of asynchronous, customized broadcast/reduction, we can reduce the dominating latency cost in sparse triangular solution. The effectiveness of these techniques will be demonstrated with our open source software STRUMPACK and SuperLU.
Anisotropic mesh adaptation using enriched reconstructed solutions

André Fortin* and Thomas Briffard

Mesh adaptation is a crucial part of modern finite element codes since it allows to control the accuracy of finite element approximations to solutions of problems with ever increasing complexity. In this talk, we present such a mesh adaptation method where we start with a finite element approximation of degree \( k \) and use gradient recovery techniques to construct an enriched solution of degree \( k + 1 \). The difference between these two approximations is used as an error indicator. Using this error indicator, the mesh is modified by local operations such as node displacement and node elimination, edge swapping and edge division. To reduce the computational cost, the domain is partitioned into subdomains and these local mesh operations are performed independently on each subdomain in parallel. The proposed method can be applied a very large class of problems where Lagrange finite elements are used. The resulting meshes can be strongly anisotropic when and where the solution allows it. Various examples, including singular or nearly singular problems, free surface problems and frictional contact problems will be presented to illustrate the performance of our method.

A Root-node Approach to Algebraic Multigrid

Luke Olson*  Tom Manteuffel  Jacob Schroder  Ben Southworth

The focus of this talk is to provide an overview of root-node-style algebraic multigrid (AMG). While standard approaches to AMG are developed for solving symmetric positive definite (SPD) systems that arise from discretizing partial differential equations, certain SPD problems, such as anisotropic diffusion, are not adequately addressed by existing methods. Non-SPD problems pose a significant challenge, and in practice AMG is often dismissed as a solver in these cases. So-called root-node AMG, which can be viewed as a combination of classical and aggregation-based multigrid, offer a potentially more robust framework in many cases.

In this talk, we outline an algorithm for root-node AMG, including a filtering strategy that controls the cost of using root-node AMG in more complex scenarios. We provide some theoretical footings for root-node AMG in the case of symmetric and non-symmetric settings. In addition, numerical results are presented demonstrating the robust ability of root-node AMG to solve nonsymmetric problems, systems-based problems, and difficult SPD problems.
Automatic Construction of AMG Smoothers

Lisa Claus*  Matthias Bolten  Robert D. Falgout

Algebraic Multigrid (AMG) is used to speed up linear system solves in a wide variety of applications. This talk is concentrated on expanding AMG’s applicability to important new classes of problems through algorithms that automatically construct advanced smoothing techniques when needed. AMG algorithms are usually designed by first assuming that the smoother is a simple pointwise smoother, then great effort is put into constructing an interpolation and corresponding coarse-grid correction that complements the smoother and leads to fast $O(N)$ convergence. The so-called weak approximation property and basic two-grid theory are used to guide algorithm development. However, for some classes of problems, pointwise smoothers are not sufficient for achieving the desired $O(N)$ computational complexity. In this talk, we use two-grid theory to motivate the development of new algorithms for automatically constructing more complex (non-pointwise) smoothers. As a relevant application, we consider a curl-curl problem that often arises in time-domain electromagnetic simulations. We use a Nédélec $H(curl)$-conforming finite element approach to discretize the problem and demonstrate how our new AMG smoother algorithms recover the well known Arnold-Falk-Winther and Hiptmair smoothers. We also discuss future directions in more general application settings.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

An Adaptive Unsmoothed Aggregation Multigrid Method Based on Path Coverings

Junyuan Lin*  Xiaozhe Hu  Ludmil Zikatanov

We propose an adaptive algebraic multigrid (AMG) method for efficient solution of linear systems with matrices derived from discretizations of second order elliptic partial differential equations or weighted Laplacians from graph problems. The overall algorithm is nonlinear and the main idea is to approximate the level sets of the smooth errors by nearly optimal path coverings and matching along the paths. Traditionally, the unsmoothed aggregation AMG (UA-AMG) methods require more sophisticated cycling techniques, such as W-cycle or K-cycle. As the numerical results show, the proposed method based on adaptive path coverings leads to an optimal V-cycle algorithm for model problems. Therefore, it is more efficient and easier to implement in practice which will have advantages in many applications.

Approximate Ideal Restriction (AIR): an Algebraic Multigrid Method for Nonsymmetric Linear Systems

Ben Southworth*  Tom Manteuffel  John Ruge  Ruipeng Li

A new algebraic multigrid (AMG) method has been developed recently based on an approximate ideal restriction (AIR), which has demonstrated potential as a fast, parallel solver for scalar hyperbolic PDEs. In this talk, we discuss the convergence properties of AIR, motivating choices in its development, and explaining the strong convergence attained on difficult scalar problems. The parallel implementation of AIR, which is now available in the hypre library, will be discussed, along with scaling and performance of different realizations of AIR. Finally, we demonstrate AIR as a tool for solving high-dimensional PDEs, or systems of PDEs, with hyperbolic character. First, we look at coupling AIR with the diffusion synthetic acceleration (DSA) approach to solving the radiative transport equation. Because AMG scales well in parallel, AIR offers better parallel scaling than a traditional transport sweep associated with the DSA
algorithm. We then look at AIR as a linear solver for full space-time discretizations, offering a new algebraic perspective on parallel-in-time.

Chair: Olof Widlund

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<td>10:30-12:30</td>
<td>MS08: Domain Decomposition preconditioners for Isogeometric Analysis Arts-1043</td>
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A domain decomposition method with fast diagonalization subdomains solvers for isogeometric discretizations

Michał Bosy∗ Monica Montardini Giancarlo Sangalli Mattia Tani

The performance of domain decomposition methods depends on the local solvers. We combine a FETI like DD approach with the fast diagonalization solver which is a fast solver on a single isogeometric patch. The fast diagonalization solver takes advantage of the tensor-structure of multivariate splines. Each application of the preconditioner is a direct solve of a suitable Sylvester-like equation. The preconditioner is robust with respect to the spline degree p and in practice has a computational cost that is independent of p and negligible with respect to the matrix-vector operations. We present numerical benchmarks that show the good performance of the proposed strategy.

Isogeometric Solvers based on Greedy Tensor Approximation Methods

Clemens Hofreither

We present a recently developed method for low-rank tensor approximation called Greedy Tucker Approximation. It can be used both to approximate directly given tensors as well as to compute approximate solutions to linear systems given in low-rank tensor format. Its core idea is the iterative, greedy selection of a suitable small tensor product subspace of the entire linear space of tensors under consideration. In each iteration, this small subspace is enriched by means of a best rank one approximation or a rank one minimizer of the residual. In this small subspace, the sought tensor is then approximated, either by orthogonal projection in the direct approximation case (algorithm GTA) or by a Galerkin or least-squares projection of the global linear system in the linear system case (algorithm GTA-LS).

We then demonstrate how tensor approximation methods can be used to construct solvers for tensor product Isogeometric Analysis. For instance, low-rank approximations of IgA stiffness matrices can be obtained by combining GTA with the reordered structured matrix format developed previously for a black-box fast IgA assembly algorithm. If an IgA stiffness matrix has sufficiently low tensor rank itself, then the resulting linear system can be directly solved by the GTA-LS method. In the more general case where the linear operator has higher rank, a low-rank approximation computed by means of GTA can be used to construct a low-rank preconditioner for the original problem which is applied by means of GTA-LS. These techniques make it possible to tackle problem sizes which are beyond the reach of standard linear algebra techniques for full-grid discretizations due to memory and computational constraints.
We propose and investigate new robust time-parallel solvers for the huge systems of linear algebraic equations arising from the time-multipatch space-time Isogeometric Analysis (IGA) discretization of parabolic initial boundary-value problems. This discretization scheme has recently been proposed by C. Hofer, U. Langer, M. Neumüller and I. Toulopoulos (2017), and is based on the stabilized singlepatch IGA discretization introduced by U. Langer, S. Moore and M. Neumüller (2016). The space-time cylinder, in which the parabolic problem is posed, is decomposed into time-slabs which are coupled via a discontinuous Galerkin technique. Each time-slab has a single or multipatch geometrical representation. The time-slabs provide the structure for the time-parallel multigrid solver proposed by M. Ganter and M. Neumüller (2016). The most important part of this time-parallel multigrid solver is the smoother. We use the special tensor structure of the involved matrices to decouple its inversion into several spatial problems by means of generalized eigenvalue or Schur decompositions. For the spatial problems, robust solvers or preconditioners are available. Finally, we present numerical experiments confirming the robustness of our space-time IgA solver.

The authors would like to express their thanks to the Austrian Science Fund (FWF) for supporting our research work under the grant W 1214-04.

Isogeometric FETI-DP methods for Almost Incompressible Elasticity

Building on previous work of Li and Tu, we will extend previous results of Pavarino and Scacchi using a FETI-DP algorithm for an Isogeometric discretization of almost incompressible elasticity in three dimensions.

Chair: Sara Pollock
10:30-12:30 MS13:Discretization and Multilevel Methods for Nonstandard FEM

Auxiliary Space Preconditioners for Virtual Element Discretization

In this talk, we will present efficient solvers for solving the linear systems of equations arising from the virtual element method (VEM) discretization of second order elliptic partial differential equations on polytopal mesh. By using the general auxiliary space framework, we design robust and efficient preconditioners for the VEM discretizations on polytopal mesh in both 2D and 3D. We will present some numerical experiments to demonstrate the theoretical results.
Weak Galerkin Method and Its Applications

Xiu Ye*  Shangyou Zhang

Newly developed weak Galerkin (WG) finite element methods will be introduced for solving partial differential equations on polygonal mesh. The weak Galerkin method is a natural extension of the standard Galerkin finite element method for the function with discontinuity where classical derivatives are substituted by weakly defined derivatives. Therefore, the weak Galerkin methods have the flexibility of employing discontinuous elements and, at the same time, share the simple formulations of continuous finite element methods.

The purpose of this presentation is to introduce some new developments of the WG methods and their applications. A robust WG method will be presented for solving the Reissner-Mindlin plate problem with uniform convergence. Also a simple WG method will be introduced to solve for singularly perturbed convection-diffusion-reaction problems. A posteriori analysis with simple estimator for WG method will also be discussed.

Stable discretizations and parameter-robust preconditioners for flux-based multiple-network poroelastic systems

Johannes Kraus*  Qingguo Hong  Maria Lymbery  Fadi Philo

Multiple-network poroelastic theory (MPET) has been introduced in geomechanics to describe the mechanical deformation and fluid flow in media with different porosities and permeabilities as a generalization of Biot’s theory (see Bai, Elsworth, and Roegiers 1993). More recently, it has also been applied successfully in the modeling of cerebral water transport (Tully and Ventikos 2011). The parameters in the governing system of partial differential equations typically vary over several orders of magnitude making its stable discretization and efficient solution a challenging task as for the case of Biot’s consolidation model (Hong and Kraus 2017; Lee, Mardal, and Winther 2017).

Here we generalize our approach of using pointwise mass-conservative discretizations for the classical three-field formulation of the single-network poroelastic problem (cf. Hong and Kraus 2017), to a flux-based formulation of multiple-network poroelastic systems. The key to establish the uniform inf-sup stability of the continuous problem is the choice of proper parameter-dependent norms. This allows also the parameter-robust transfer of the induced norm-equivalent preconditioners to the discrete level. We further prove the corresponding optimal error estimates.
Coupling hydrostatic and nonhydrostatic Navier-Stokes flows using a Schwarz algorithm

Eric Blayo* Antoine Rousseau

In the context of ocean modeling, almost all circulation models, either at large scale or at regional scale, are based on the so-called *primitive equations*, which make use of the hydrostatic approximation. However continuous improvement in numerical modeling and in computing resources leads to more and more sophisticated ocean modeling systems, which aim at representing the full ocean physics. A natural idea is thus to build systems that couple local nonhydrostatic models to larger scale hydrostatic ones. Such a coupling is quite delicate from a mathematical point of view, due to the different nature of hydrostatic and nonhydrostatic Navier-Stokes equations (where the vertical velocity is either a diagnostic or a prognostic variable). In this talk, we propose to couple such systems through a Schwarz iterative algorithm, and we look for relevant interface conditions that would both lead to a well posed coupled problem and minimize the computational cost.

Coupled Parareal-Optimized Schwarz Waveform relaxation method for advection reaction diffusion equation

Duc-Quang Bui* Caroline Japhet Yvon Maday Pascal Omnes

Parareal method is a numerical method to solve time - evolutional problems in parallel, which uses two propagators: the coarse - fast and inaccurate - and the fine - slow but more accurate. Instead of running the fine propagator on the whole time interval, we divide the time space into small time intervals, where we can run the fine propagator in parallel to obtain the desired solution, with the help of the coarse propagator and through parareal steps. Furthermore, each local subproblem can be solved by an iterative method, and instead of doing this local iterative method until convergence, one may perform only a few iterations of it, during parareal iterations. Propagators then become much cheaper but sharply lose their accuracy, and we hope that the convergence will be achieved across parareal iterations.

In this talk, we propose to couple Parareal with a well-known iterative method - Optimized Schwarz Waveform Relaxation (OSWR) - with only few OSWR iterations in the fine propagator and with a simple coarse propagator deduced from Backward Euler method. We present the analysis of this coupled method for 1-dimensional advection reaction diffusion equation, for this case the convergence is almost linear. We also give some numerical illustrations for 1D and 2D equations, which shows that the convergence is much faster in practice.

A posteriori error estimates and stopping criteria for space-time domain decomposition for two-phase flow with discontinuous capillary pressure

Michel Kern* Elyes Ahmed Sarah Ali-Hassan Caroline Japhet Martin Vohralík

We consider two-phase flow in a porous medium composed of different rock types, so that the capillary pressure field is discontinuous at the interface between the rocks and creates a capillary trap for oil or
gas. This is a nonlinear and degenerate parabolic problem with nonlinear and discontinuous transmission conditions on the interface. The problem is solved by a space–time domain decomposition (DD) method based on the Optimized Schwarz Waveform Relaxation algorithm (OSWR) with Robin or Ventcell transmission conditions. Space-time subdomain problems across the time interval are solved at each OSWR iteration, and the exchange between the subdomains uses time-dependent and higher order transmission operators. Numerical approximation is achieved by a finite volume scheme, using the Matlab Reservoir Simulation Toolbox. We then show how a posteriori error estimators, based on reconstruction techniques for pressures and fluxes, lead to efficient stopping criteria for the DD iterations. The estimators are split into different components corresponding to the space and time discretization errors, and to the errors due to the Newton linearization and the DD iterations. The DD iterations can be stopped as soon as the DD estimator becomes smaller than the discretization estimators.

### Analysis of overlap in optimized waveform relation methods for RLCG transmission line type circuits

Pratik M. Kumbhar*, Martin J. Gander

Among many applications of parallel computing, solving large systems of ordinary differential equations (ODEs) which arise from large scale electronic circuits, or discretizations of partial differential equations (PDEs), form an important part. A systematic approach for their parallel solution are Waveform Relaxation (WR) techniques, which were introduced in 1982 for circuit solver applications. These techniques are based on partitioning large circuits into smaller sub-circuits, which are then solved separately over multiple time steps, and the overall solution is obtained by an iteration between the sub-circuits. However, this technique can lead to non-uniform and potentially slow convergence over large time windows. To overcome this issue, optimized waveform relaxation techniques were introduced, which are based on optimizing a parameter. We show how this method improves the convergence for RLCG transmission line type circuits. We introduce overlap between sub circuits and analyze its effect on the convergence factor. For R=0, we find that these RLCG circuit equations represent discretizations of the well known Maxwell equations. We relate these two models and give some asymptotic results.

Chair: Hormoz Jahandari
10:30-12:30 Contributed Talks Arts-2071

### A coupled acoustic-elastic wave solver for estimating seismic amplitudes

Ligia Elena Jaimes Osorio, Alison Malcolm*

Variation in seismic amplitude with changes in distance between source and receivers is typically associated with changes in fluid content in rocks above and below discontinuities in subsurface material parameters. When studying these amplitude variations either plane waves or spherical waves simulation methods are used. Spherical waves methods such as full waveform inversion better model the reflection amplitude, since these handle near and post-critical reflections, are applicable to heterogeneous models and iteratively invert for multiple parameters, but, these methods are time and computationally expensive. Often, in characterization of reservoirs the interest is focused in a limited subsurface area. To avoid the use of an
expensive full domain elastic solver, we use a coupled acoustic-elastic (CDA-EL) solver to model these effects. In this method, an acoustic solver is used to propagate the wavefield to a subdomain in which a local elastic solver is implemented, incorporating elastic physics in the region of interest. Once the amplitude of the local reflector is calculated, we proceed to investigate if we can use these data to invert for the material properties at a reflector of interest.

A time adaptive multirate Neumann-Neumann waveform relaxation method for heterogeneous coupled heat equations

Azahar Monge∗ Philipp Birken

The efficient simulation of thermal interaction between fluids and structures is crucial in the design of many industrial products, e.g. thermal anti-icing systems of airplanes, gas quenching, which is an industrial heat treatment of metal workpieces or the cooling of rocket thrust chambers. Unsteady thermal fluid structure interaction is modelled using two partial differential equations describing a fluid and a structure which are coupled at an interface. The standard algorithm to find solutions of the coupled problem is the Dirichlet-Neumann iteration, where the PDEs are solved separately using Dirichlet, respectively Neumann boundary with data given from the solution of the other problem. Previous analysis and numerical experiments show that this iteration is fast for the thermal coupling of air and steel [A. Monge and P. Birken, On the convergence rate of the Dirichlet-Neumann iteration for unsteady thermal fluid-structure interaction. Comp. Mech., Online First 2017]. This method has two main disadvantages: the subsolvers are sequential and both fields are solved with a common time resolution. Using instead a time adaptive multirate scheme would be more efficient. In view of this, we present here a high order, parallel, time adaptive, multirate numerical method for two heterogeneous coupled heat equations. We use the Neumann-Neumann waveform relaxation (NNWR) method which is a variant of WR methods based on the classical Neumann-Neumann iteration [M. J. Gander, F. Kwok and B. C. Mandal, Dirichlet-Neumann and Neumann-Neumann waveform relaxation algorithms for parabolic problems. ETNA, Vol. 45, pp. 424–456, 2016]. When choosing the relaxation parameter right, two iterations are sufficient. We present an analysis of the NNWR algorithm that shows that the optimal relaxation parameter is highly dependent on the material coefficients. In order to get an adaptive multirate scheme, we use possibly different adaptive temporal discretization methods on the two subdomains. Furthermore, two time integration alternatives are analyzed, the implicit Euler method and a second order singly diagonally implicit Runge-Kutta method (SDIRK2). Numerical results show that second order is achieved even when using linear interpolation in the multirate case.

Enabling physics-based domain decompositions in environmental applications through a flexible software ecosystem

J. David Moulton* A. Jan E. T. Coon S. L. Painter

The increasing need to understand and predict climate impacts and feedbacks in terrestrial systems is creating challenges in multiscale and multiphysics modeling. Managing the complexity of these process-rich integrated hydrologic models requires flexible software designs that enable exploration of model features and model coupling. To address this need the Interoperable Design of Extreme-Scale Application Software (IDEAS) project is exploring new-community based approaches to establishing a flexible and extensible software ecosystem of interoperable components that can be shared between applications and composed in novel ways. An important implication of this approach is that it provides modelers with tools to develop physics-based decompositions and sub-grid models from existing components, and test their efficacy directly against the higher-fidelity fine-scale models. In this talk we demonstrate these concepts using a mixed-
dimensional model structure for efficiently simulating surface/subsurface thermal hydrology in low-relief permafrost regions at watershed scales using the Advanced Terrestrial Simulator (ATS) and its multiphysics framework dubbed Arcos. The approach replaces a full three-dimensional system with a two-dimensional overland thermal hydrology system and a family of one-dimensional vertical columns, where each column represents a fully coupled surface/subsurface thermal hydrology system without lateral flow. The Arcos framework makes this approach tractable, automating the creation and temporal evolution (sub-cycling) of the one-dimensional columns within the mixed-dimensional approximation. The efficacy of this approach is demonstrated through numerical simulations of a site in Barrow, AK, which are the first advanced representations of freezing soil physics coupled to overland thermal flow and surface energy balance at scales of 100s of meters. In addition, we show that the Arcos framework design naturally supports the development of subgrid models for water retention and routing due to microtopography, and aids in the characterization of parameters in these models.

**A finite element nonoverlapping domain decomposition method with Lagrange multipliers for the dual total variation minimizations**

Chang-Ock Lee  Jongho Park*

Total variation regularization is a standard technique for variational image processing. In this talk, we consider a primal-dual domain decomposition method for the total variation regularized problems. The Fenchel-Rockafellar dual of the model problem is transformed into an equivalent constrained minimization problem by tearing-and-interconnecting domain decomposition. Then, the continuity constraints on the subdomain interfaces are treated by introducing Lagrange multipliers. The resulting saddle point problem is solved by the first order primal-dual algorithm. We apply the proposed method to image denoising, inpainting, and segmentation problems with either $L^2$-fidelity or $L^1$-fidelity. Numerical results are presented.

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Thoughts on Composing Nonlinear Solvers

Matthew Knepley*

We present, in analogy with the linear preconditioning operation, a framework for the composition of nonlinear solvers, which we call nonlinear preconditioning, in order to accelerate convergence and improve solver performance. A central problem for this operation is that no rules of thumb exist for choosing the operations or composition strategy, and theory has been an unreliable guide. We explore a possible alternative, the nondiscrete induction of Ptak, which could allow us to understand the short time behavior of composed iterations.
An algebraic view on BDDC - from local estimates to eigenvalue problems, parallel sums, and deluxe scaling

Clemens Pechstein*

In this talk (joint work with Clark Dohrmann, Sandia labs), a theoretical framework on (adaptive) BDDC / FETI-DP is exposed that applies to general symmetric positive definite problems. We show how the central estimate related to the average operator can be localized to globs, i.e. faces, edges, vertices of the subdomain decomposition, and how an overall reliable condition number bound can be obtained. We also compare with other approaches in the literature.

The best constant in every such local estimate can be obtained by regarding an associated generalized eigenvalue problem. The relevant extremal eigenvalue can be improved by deflating against the first few eigenvectors. We show how these deflations vectors can be turned into regular primal constraints and as such lead to an adaptively chosen coarse space. Sometimes it is advantageous to simplify the generalized eigenvalue problems. For globs shared by two subdomains, the number of unknowns can be reduced by a factor of two using the parallel sum of matrices introduced by Anderson and Duffin. Matters are more difficult if a glob is shared by three or more subdomains. We discuss several ways how to simplify the eigenvalue problems and relate again to other approaches in the literature.

So far we have not assumed any specific choice of the weighting matrices that define the average operator. We show that the deluxe scaling is again related to the parallel sum of matrices and that it satisfies a certain optimality property.
BDDC Deluxe Algorithms for Isogeometric Analysis and Linear Elasticity

Olof B. Widlund* Luca F. Pavarino Simone Scacchi Stefano Zampini

A survey will be given of recent work on BDDC Deluxe algorithms for linear elasticity. This work is joint with Luca Pavarino, Simone Scacchi, and Stefano Zampini. Our choice of domain decomposition algorithms is inspired by the considerable success of this variant of the BDDC algorithm for scalar elliptic problems in two and three dimensions. The analysis of three dimensional elasticity has led to development of several new technical tools among them a new face lemma. Our studies concern compressible elasticity as well as the almost incompressible case. The latter is inspired by an excellent 2015 SINUM paper by Xuemin Tu and Jing Li on mixed finite elements.

Chair: Daniel Szyld

10:30-12:30 MS12:Asynchronous Domain Decomposition Methods Arts-1045

Asynchronous Optimized Schwarz Methods for Poisson’s equation in rectangular domains

Jose Garay* Frédéric Magoulès Daniel Szyld

Optimized Schwarz methods (OSM) are domain decomposition methods that are fast in terms of iteration count and can be implemented asynchronously. These two properties make of OSM potentially good methods for the solution of PDEs using modern supercomputers. In this presentation we analyze the convergence of OSM applied as solvers for the solution of Poisson’s equation in rectangular domains. The subdomains are also rectangles, and our analysis includes the case of cross points. We assume that the (physical) boundary conditions are of Dirichlet type, and those on the artificial interfaces are of Robin type. We study the synchronous and asynchronous implementations of the method. Numerical experiments results illustrate our theoretical results.

Performance of Asynchronous Optimized Schwarz on a Distributed-memory Computer

Ichitaro Yamazaki* Edmond Chow Jack Dongarra

To address the increasing cost of the synchronization, we study the performance of the asynchronous optimized Schwarz method on a distributed-memory computer. Though the performance of the method has been previously studied, the previous studies focused on the convergence and the potential of the asynchronous method to improve the performance of the synchronous method. Since the asynchronous method more likely outperforms the synchronous method when the load imbalance among the processes or the non-uniformity in the hardware performance exists, the previous experiments were conducted using irregular meshes on the heterogeneous distributed-memory computer that has different CPUs on each node. To study both the potential and the limitation of the asynchronous method on the current and future distributed-memory computers, in this talk, we study their performance with 2D regular meshes that are evenly partitioned among the processes on the current leadership supercomputer.
Asynchronous Domain Decomposition Solvers

Christian Glusa

Parallel implementations of linear iterative solvers generally alternate between phases of data exchange and phases of local computation. Increasingly large problem sizes on more heterogeneous systems make load balancing and network layout very challenging tasks. In particular, global communication patterns such as inner products become increasingly limiting at scale.

In this talk, we explore the use of asynchronous domain decomposition solvers based on one-sided MPI primitives. We will discuss practical issues encountered in the development of a scalable solver and show experimental results obtained on a variety of state-of-the-art supercomputer systems.

Chair: Felix Kwok
10:30-12:30
MS15:Advances in Schwarz waveform relaxation and space-time DD methods

Resistive Coupling based Waveform Relaxation for Analysis of Transmission Line Circuits

Tarik Menkad* Anestis Dounavis

Extending the optimized waveform relaxation methods introduced by Gander et al. for the time-domain analysis of RC diffusive circuits and one single line problem, to more general two-conductor transmission line (TL) circuits, requires a new approach to the traditional questions of partitioning and fast convergence. First, the distributed nature of the transmission lines must be preserved, and the partitioning strategy has to apply with any time-domain line macromodeling algorithm. The proposed partitioning scheme uses node tearing and adds an external circuit implementation of the transmission conditions at the boundary between every two adjacent sub-circuits. The added resistive interface provides the necessary overlap to decouple sub-circuits, and preserves the distributed nature of a transmission line. It does not alter the solution of the Whole system.

Second, fast WR convergence is cast as a bundle optimization of all the interdependent local convergence rates of WR for a multi-subsystem partition. A direct numerical solution would not be cost-effective and alternative methods are required. The minmax companion problem is solved here in a suboptimal sense; a nearby minmax problem is defined and numerically solved on a small and apriori known number of instances, which scales linearly with the size of the partition. Suboptimal values for the relaxation resistances are computed at a low cost.

A WR algorithm is presented, it uses the proposed system partitioning and the resistive based relaxation for the time-domain analysis of general TL circuits. The Gauss Seidel iteration of this WR algorithm is executed with a basic scheduling. Numerical examples show that the parallel implementation of this WR algorithm outperforms direct solvers in the analysis of TL arborescent circuits.
Discrete Schwarz Waveform Relaxation Analysis of Rosenbrock Methods for the Heat equation

Khaled Mohammad* Ronald D. Haynes

A class of linearly implicit Schwarz waveform relaxation methods based on Rosenbrock time integrators are proposed and analyzed at the discrete level. We discuss the sufficient conditions for the convergence of Schwarz waveform relaxation algorithm at the discrete level for the Rosenbrock type methods. We show that the classical Schwarz waveform relaxation algorithm does not converge for certain forms of Rosenbrock methods. We use the discrete Laplace transform to prove the convergence of the overlapping Rosenbrock Schwarz waveform relaxation algorithm for the Heat equation on two subdomains and multiple subdomains.

Nested Schwarz Waveform Relaxation for Time-Fractional PDEs in 2D

Shu-Lin Wu* Yingxiang Xu

In the study of Schwarz waveform relaxation (SWR) algorithms, asymptotic convergence analysis is an important work and the result mainly reveals how the convergence factor behaves when both the spatial and temporal mesh sizes approach to zero in certain manner, i.e., \( \rho = 1 - O(\Delta x^\alpha) \) when \( \Delta t = O(\Delta x^\beta) \) and \( \Delta x \to 0 \), where \( \alpha \geq 0 \) and \( \beta > 0 \) are constants. The main purpose of this talk is to discuss how to further use such an asymptotic result. In particular, following the idea of Hackbusch, we show that a nested version of the SWR algorithms can be established, which results in optimal computational complexity in practice. Precisely, we first make several levels of spatial grids denoted by \( \Delta x_1 < \Delta x_2 < \cdots < \Delta x_L \); then on the \( m \)-th grid level we run the SWR algorithms for \( k_m \) iterations and then the obtained solution is prolonged to the \((m - 1)\)-th grid level as the initial guess for the SWR algorithm on this less coarse grid level. On the coarsest grid level, i.e., the \( L \)-th level, we solve the underlying PDE directly. Interestingly, there exists best choice of the integers \( \{k_{L-1}, k_{L-2}, \ldots, k_2, k_1\} \), i.e., the iteration number fixed for each grid level, which minimize the computational complexity. We will show details about how these iteration numbers depend on the quantity \( \alpha \). We will illustrate the theoretical and numerical results for the time-fractional PDEs in 2D, for which both the classical transmission conditions (TCs) of Robin type and the optimal TCs of convolution type are studied.

Chair: José Pablo Lucero Lorca

10:30-12:30 MS16: Solvers and preconditioners for non-conforming discretization methods

Multigrid algorithms for discontinuous Galerkin methods on polytopic grids

Paola F. Antonietti Giorgio Pennesi*

We present a V-cycle multigrid solver for the numerical solution of the linear systems of equations arising from discontinuous Galerkin discretizations of second-order elliptic partial differential equations on polygonal/polyhedral meshes. Here, the sequence of spaces that stands at the basis of the multigrid scheme is
possibly non nested and is obtained based on employing agglomeration techniques with edge/face coarsening. We prove that the V-cycle scheme converges uniformly with respect to the granularity of the grid and the polynomial approximation degree, provided that the number of Richardson smoothing steps is chosen sufficiently large. We improve the convergence properties of the method by defining a domain decomposition preconditioner that we use as a smoothing operator. A series of numerical tests are presented in order to validate the theoretical results.

A Balancing Domain Decomposition by Constraints Preconditioner for $C^0$ Interior Penalty Methods

Kening Wang* Susanne C. Brenner Eun-Hee Park Li-Yeng Sung

A balancing domain decomposition by constraints (BDDC) algorithm is constructed and analyzed for a discontinuous Galerkin method, the $C^0$ interior penalty method, for biharmonic problems. The condition number of the preconditioned system is bounded by $C(1 + \ln(H/h))^2$, where $h$ is the mesh size of the triangulation, $H$ is the typical diameter of subdomains, and the positive constant $C$ is independent of $h$ and $H$. Numerical experiments corroborate the theoretical result.

Discrete Duality Finite Volume methods on a subdomain of a non-convex domain

Sandie Moody* Martin J. Gander

This work originated from a collaboration with the Swiss weather prediction service MeteoSwiss, and we thus restrict ourselves to a specific domain and grid. We look to solve a diffusion problem on this domain. The domain considered is polygonal and presents a reentrant corner. It can be split into two subdomains, one of which contains the reentrant corner. We define a regular grid on the subdomain which does not contain the reentrant corner and implement a standard finite volume method to solve the diffusion problem there. On the other subdomain, the grid is not admissible for the standard finite volume method, and we thus use instead a discrete duality finite volume method. At the interface, a coupling of both methods is implemented. The subdomain containing the reentrant corner can itself be decomposed into subdomains which will be refined differently whether they contain the reentrant corner or not, in order to compensate for the loss of regularity of the solution near the reentrant corner. This coupling method on the refined grid allows us to recover the optimal order of convergence at reduced costs.

A nonlinear multilevel Schwarz preconditioner for a discontinuous Galerkin discretization of transport equations in local thermodynamic equilibrium.

José Pablo Lucero Lorca* Guido Kanschat

We present a multigrid preconditioned, asymptotic preserving, weakly penalized discontinuous Galerkin method using nonoverlapping Schwarz smoothers to solve a frequency and angle dependent radiative transfer equations with applications in particle transport through diffusive media. Frequencies and angles are discretized by multigroup and collocation, respectively. We use a nonlinear additive Schwarz method to precondition the Newton solver. By solving full local radiative transfer problems for each grid cell, performed in parallel on a matrix-free implementation, we achieve a method capable to address large scale calculations arising from applications such as astrophysics, atmospheric radiation calculations and nuclear applications.
In several tests we show the robustness of the approach for different mesh sizes, cross sections, frequency distributions and anisotropic regimes.

Instability-effects of a localization-method for nonlinearities in dual domain-decomposition and use of recycling methods

Andreas S. Seibold*  Michael Leistner  Daniel J. Rixen

Over the last years several approaches and works have been published on localization methods for nonlinear domain-decomposition, such as FETI, BDD and mixed formulations. These localization methods aim to improve parallelity of the solution process by concentrating computational effort on processor cores and reducing global iterations. This is achieved by local Newton-Raphson iterations on each substructure, while a global nonlinear iterative solver is responsible for the exchange of information between substructures [Gosselet, P. et al. “Substructured formulations of nonlinear structure problems - influence of the interface condition”. In: International Journal for Numerical Methods in Engineering (2015)], [Klawonn, A., Lanser, M., Rheinbach, O., and Uran, M. “Nonlinear FETI-DP and BDDC Methods: A Unified Framework and Parallel Result”. In: SIAM Journal on Scientific Computing 39.6 (2017), pp. C417–C451]. Besides, recycling-methods have been developed to improve the FETI-solver’s efficiency, such as adaptive multipreconditioning and Total Reuse of Krylov Subspaces [Leistner, M., Rixen, D., and Gosselet, P. “Application of Multipreconditioned Iterative Algorithms in Dual Domain Decomposition Methods for Structural Dynamics”. In: PAMM (2017)]. In our study, we examine the behaviour of the above described localization technique in combination with a dual FETI-2-solver in terms of stability issues in bending-cases and badly shaped subdomains. Furthermore we augmented the FETI-solver with recycling-methods for the dual solutions and discovered interesting behaviour of the global solver. In cases of static instabilities, such as buckling, the localized solver loses its advance compared to a standard Newton-Krylov-Schur solver and needs even more iterations. With recycling methods this disadvantage can be approximately equalized. Especially new recycling-methods approximating GenEO-modes with Ritz-vectors show good results while using a smaller subspace. Other convergence preventing instability effects are related to inhomogeneous deformations on the interfaces due to lower local stiffnesses leading to high rotational displacements of such substructures. These cannot be balanced by the FETI-solver. The proposed modification to the localization method and to the FETI-2 strategy will be discussed and illustrated on some academic examples.

Conjugate gradient for nonsingular saddle-point systems with a highly singular leading block

Michael Wathen*

We consider iterative solvers for large, sparse, symmetric linear systems with a saddle-point structure. Since such systems are indefinite, the conjugate gradient (CG) method cannot typically be used. However, in the case of a maximally rank-deficient leading block, we show that there are two necessary and sufficient conditions that allow for CG to be used. We show that the conditions are satisfied for a model mixed
Maxwell problem. To support our analysis, we present several three-dimensional numerical experiments on complicated computational domains or with variable coefficients.

**A coupling simulation for the multilevel radiative diffusion equation based on the domain decomposition method**

Rong Yang∗ Xudeng Hang

Radiation multigroup diffusion equation and radiation heat conduction equation are usually used in transport theory research and numerical simulation. In this paper we present an approach to simulate the coupling model of multigroup radiation diffusion and heat conduction. Typically a domain decomposition is done by an iteration procedure at each time step, in which the multigroup diffusion and the heat conduction equation are solved through an interface condition which provides the boundary conditions for each subdomain, alternately until convergence of the successive approximation is reached. The two new interface conditions are obtained separately based on the flux or temperature continuousness across the interface. The algorithm is implemented in two-dimensional Radiation Hydrodynamics Code Lared-R. The transfer tube and implosion problems of Inertial Confinement Fusion (ICF) are tested and the results demonstrate the good effect of the coupling simulation on the computing efficiency as well as accuracy. Also the effect of the coupling simulation by the different interface conditions are discussed.
Stability Analysis of Inline ZFP Compression for Floating-Point Data in Iterative Methods

Alyson Fox

ZFP [Lindstrom and Isenburg, Fast and efficient compression of floating-point, IEEE Transactions on Visualization and Computer Graphics (2014)], a state-of-the-art lossy compression algorithm, can easily be used inline during numerical simulations due to the inherent locality of the algorithm. ZFP decomposes a solution state into 4d blocks, which are subsequently compressed independently. Similarly, decompression is performed on each independent block. In a numerical simulation, the solution state already contains traditional errors, e.g., floating-point round-off, truncation error, and discretization error. The information that is lost during ZFP compression may represent the traditional errors, however, any additional error caused by ZFP could contaminate the current iterate. It is important to understand if the error from ZFP compression overwhelms the other sources of error. The goal of this work is to analyze the stability of using ZFP in fixed precision inline in time-evolving iterative methods. We introduce the infinite bit vector space and define corresponding operators for each step of ZFP, to establish an error bound for both a static and iterative implementation of ZFP in fixed precision. In particular, we establish stability results for Lipschitz-continuous operators (linear or nonlinear) and Kriess-bounded linear operators.

Solving High-order Discretizations of Thermal Radiative Transport

Terry Haut  Peter Maginot  Ben Southworth  Vladimir Tomov

Thermal radiative transfer (TRT) is a critical but expensive component of large-scale multi-physics simulations. TRT can require upwards of 40K unknowns per spatial zone, and may account for 90% of a multi-physics simulation’s total runtime. High-order (HO) discontinuous finite elements (DFEM) offer great promise for better physics fidelity as well as reducing the number of degrees-of-freedom required for multi-physics simulations. However, using HO finite elements and corresponding HO meshes introduce new challenges for solving the radiative transport equations. Here, we present numerical methods for solving HO DFEM discretizations of TRT. The primary difficult with HO discretizations of TRT is that HO meshes lead to "cycles" in the mesh, and the associated linear system for radiative transport, in a fixed direction, is no longer block triangular. In this case, a traditional transport sweep in the context of diffusion synthetic acceleration (DSA) preconditioning breaks down. We propose several solutions, including (i) breaking the cycles and performing a block Gauss-Seidel-type iteration to solve the scalar transport equations in DSA, (ii) doing a traditional transport sweep, but identifying the strongly connected components and inverting them directly, and (iii) applying AMG in place of a transport sweep, where the triangular structure is no longer necessary.

SPMR: a Family of Saddle-Point Minimum Residual Solvers

Chen Greif

SPMR is a new family of methods for iteratively solving saddle-point systems using a minimum or quasi-
minimum residual approach. The basic mechanism underlying the method is a novel simultaneous bidiagonalization procedure that yields a simplified saddle-point matrix on a projected Krylov-like subspace, and allows for a monotonic short-recurrence iterative scheme. We develop a few variants, demonstrate the advantages of our approach, derive optimality conditions, and discuss connections to existing methods. Numerical experiments illustrate the merits of this new family of methods.

**A monotonicity-preserving multigrid algorithm for solving the equidistributing meshes in 1D**

Dawei Wang

The concept of equidistribution plays an important role in the generation of adaptive meshes, the application of which requires the solution of a boundary value problem governed by a variable-coefficient diffusion equation that is usually solved numerically in practice. However, due to the lack of connection between a priori error estimates for the numerical algorithm and mesh quality, early termination of a numerical scheme may lead to a tangled approximation of an analytically untangled mesh.

Focused on the computation of 1D equidistributing meshes as a starting point, this work tries to resolve the above problem by requiring the numerical algorithm to preserve monotonicity at every iteration. We show that the weighted Jacobi method with a suitable relaxation parameter and the Gauss-Seidel method can both preserve monotonicity of the solution at every iteration. Inspired by the algebraic multigrid (AMG) method on Markov chains, we reformulate the original problem into increment form, and transform the requirement on monotonicity to positivity. With the application of a modified multiplicative-form AMG to this system, we prove that positivity can be preserved at each iteration and every grid level (including the relaxation and coarse-grid correction steps). Therefore, the resulting meshes generated by this algorithm can not be tangled. In addition, numerical results show that this scheme gives convergence typical of AMG applied to diffusion problems.

**Convergence of classical Schwarz method for the 2-dimensional Maxwell’s equations**

Fabrizio Donzelli

This poster presents the proof of the convergence of the classical Schwarz method applied to the two-dimensional Maxwell’s equation $\Delta u - i\omega u = f$, based on the adaptation of the proof originally introduced by Schwarz in his famous example, and then generalized by Lions to more general geometries. The poster will also present another elegant proof of Lions, based on the method of orthogonal projections in Sobolev subspaces. We show that the method of projection is not, at least in an obvious way, reproducible in the case of the two-dimensional Maxwell’s equations.

**On the scalability of classical one-level domain-decomposition methods**

Faycal Chaouqui  Gabriele Ciaramella  Martin J. Gander  Tommaso Vanzan

One-level domain decomposition methods are in general not scalable, and coarse corrections are needed to obtain scalability. It has however recently been observed in applications in computational chemistry that the classical one-level parallel Schwarz method is surprisingly scalable for the solution of two-dimensional chains fixed-sized subdomains. In this poster we analyze the scalability of the parallel Schwarz method, the Optimized Schwarz method, the Dirichlet-Neumann method and the Neumann-Neumann method. In particular, the one-level domain decomposition methods are not scalable in one-dimension but scalability
is attained in two-dimensions for specific geometry and boundary conditions. Our theoretical results are illustrated by numerical experiments.

**Domain Decomposition of Mixed Finite Element Method in ESPRESO**

Lukas Maly

We propose the domain decomposition method for mixed finite element formulation of linear elasticity based on the tangential-displacement and normal-normal-stress continuous (TDNNS) elements developed by Schoeberl and Pechstein. Presented formulation of linear elasticity has wide use since the TDNNS elements are locking-free with respect to volume and shear locking, and thus they are applicable for both nearly incompressible materials and thin structures. Due to the high number of degrees of freedom and ill-conditioned system matrices arising from mixed elements, we need to apply domain decomposition methods such as FETI or primal method of Schur complement. We present an effective implementation of these methods and parallel preconditioner implemented in the in-house library ESPRESO developed at the IT4Innovation National Supercomputing Center. The poster will present a brief introduction, implementation, numerical results, and a discussion.

**Domain decomposition method for the Baltic Sea model based on theory of inverse problems and adjoint equation**

Natalia Lezina

In some problems of mathematical modeling, complex geometry of domain may be presented as a set of essentially simpler subdomains. Formulation of domain decomposition method for problems of ocean thermo-hydrodynamics suggested in [1] based on optimal control approach. In each subdomain the system of thermo–hydrodynamic equations in the Boussinesq and hydrostatic approximations is solved. The solutions in the subdomains coincide on the boundary that allow one to create iterative algorithm. The problem is how to combine solutions in subdomains into solution of the whole domain. In this case for this problem adjoint equation method and inverse problem theory are used. Also this method could be applied together with some known methods, for example, variational data assimilation [2]. Domain decomposition method for the Baltic Sea model is numerically studied. The numerical experiments with using and without domain decompositions algorithm are presented and discussed.

**A generic framework for Schwarz decomposition methods**

Pratik Nayak  Hartwig Anzt

This work concerns the study of the Schwarz decomposition methods and aims to develop a generic framework to study them. The main aim is to use the finite element framework to be able to have a mathematical basis to generate matrices from physical problems and also to apply custom boundary conditions (For the Optimized Schwarz method) for experimentation. We use the finite element library, deal.ii to be able to solve such problems. We test this framework with the Restricted additive Schwarz methods and the Optimized Schwarz methods. Future work would include adaptive mesh refinement and efforts to avoid the re-assembly of the global matrices after re-meshing. We also would like to use asynchronous communication between the different subdomains and hence an asynchronous communication.
layer is also needed. With the help of this framework, we hope to solve large scale problems in an efficient fashion with the physics of the problem kept in mind.

**A new approach for preconditioning discontinuous Galerkin discretizations**

Soheil Hajian

Domain decomposition preconditioners and in particular the additive Schwarz method are favorite preconditioners for classical finite element methods (FEM). There is a huge effort in designing similar preconditioners for discontinuous Galerkin (DG) discretizations. It has been shown that additive Schwarz methods use different mechanism for convergence when applied to a DG discretization compared to the classical FEM. More precisely, additive Schwarz methods, when applied to DG, use a non-overlapping Robin transmission condition for the communication between subdomains. This is exactly the same transmission condition that optimized Schwarz methods (OSM) use to obtain fast convergence. In this poster we present an OSM preconditioner for a particular DG discretization along with theoretical convergence estimates.

**A Reynolds Number Dependent Convergence Estimate for the Parareal Algorithm**

Martin J. Gander  Thibaut Lunet

In the attempt of achieving parallelism by decomposing the solution of one problem into several subproblems, recent efforts have been focusing on adding time as a new direction of parallelization. Among all existing timeparallel algorithms, the Parareal algorithm [Lions et al., 2001] remains one of the simplest and most prominent ones to decompose the time domain. The Parareal algorithm has favorable convergence properties when applied to parabolic problems (e.g. heat equation type), but its convergence when applied to hyperbolic problems (e.g. advection or wave equation) is not as good. In order to quantify Parareal efficiency, linear convergence bounds have been obtained in [Gander & Vandewalle, 2007] for the diffusion and the advection equation, which explain the good and not so good convergence properties of the algorithm. However, many applications (e.g. the Navier- Stokes equations) consist of a mix of those two problems, with a Reynolds number representing the ratio between the advective and diffusive terms in the equation.

We present a new linear convergence estimate for the advection-diffusion equation, depending on the Reynolds number, which characterizes accurately the depreciation of the Parareal convergence rate when the Reynolds number increases. We illustrate our new convergence estimate with numerical experiments.

**Multilevel Optimized Schwarz Methods**

Martin J. Gander  Tommaso Vanzan

Optimized Schwarz methods (OSMs) are domain-decomposition methods based on enhanced transmission conditions which are optimized in order to accelerate the convergence. We introduce a multilevel optimized Schwarz method where the transmission conditions are tuned not to improve the convergence behaviour but instead the smoothing property of the iterative scheme on each grid. We present a convergence analysis both with overlap and without overlap in a two-level setting, which also suggests how to choose the optimized parameters. Numerical results show the effectiveness of our approach both compared to the
Domain decomposition method for the Baltic Sea model based on theory of inverse problems and adjoint equation

Valery Agoshkov    Natalia Lezina

In some problems of mathematical modeling, complex geometry of domain D may be presented as a set of essentially simpler subdomains. In this subdomains, one can obtain the results of simulations, using fine meshes to achieve better approximation of boundary, bottom topography etc. To use domain decomposition methods allows one to solve problems in D subsequently solving subproblems in subdomains. New methodology for constructing the domain decomposition algorithms suggested in this work is based on the theory of optimal control, the results of the theory of inverse and ill-posed problems and the application of adjoint equations. To solve subproblems in each subdomains interface conditions are to be set. Some of them become ”controls” and are to be found with the solution in subdomains. Thus optimal control problem is obtained and could be solved with the help of already known methods. This methodology is applicable to problems with operators of different types, orders and with a different number of independent variables. The work is based on [1].

The work was supported by the Russian Science Foundation (project 14–11–00609).

New Coarse Corrections for Optimized Restricted Additive Schwarz Using PETSc

Serge Van Criekingen    Martin J. Gander

Additive Schwarz Methods (ASM) are implemented in PETSc’s PCASM preconditioner tool. By default, however, PCASM applies the Restricted Additive Schwarz (RAS) method because of better convergence behavior. We present here two further improvements for this method: a new and more effective coarse correction, as well as optimized transmission conditions, resulting in an Optimized 2-level Restricted Additive Schwarz method.

It is well known that domain decomposition methods applied to elliptic problems need a coarse correction to be scalable, since without it, information is only transferred from each subdomain to its direct neighbors which makes the number of iterations grow with the number of subdomains. Scalability is achieved by introducing a coarse grid on which a reduced-size calculation is performed, yielding a coarse correction at each iteration of the solution process. Such a 2- level method permits global propagation of the iterative corrections throughout the entire domain, leading to the scalability of the method. Many choices for the coarse grid point locations are possible and all lead to scalable methods, provided coarse grid points lie in each of the subdomains. However, a good choice of coarse grid point locations can lead to much faster methods. We follow here the method introduced in [M.J. Gander, L. Halpern and K. Santugini, A New Coarse Grid Correction for RAS/AS, Domain Decomposition Methods in Science and Engineering XXI, LNCSE, Springer-Verlag, 2014]. The coarse grid points are placed in the overlap and chosen in 1D to be the extreme grid points of the non-overlapping subdomains used to define RAS. Similarly, for a rectangular decomposition in 2D, four coarse grid points are placed around each cross point of the non-overlapping decomposition of RAS. This choice is based on approximating what is called an optimal coarse space which leads to convergence of the 2-level method in a finite number of iterations. Our choice of placing the coarse grid nodes leads to substantially faster convergence than the classical option of equally distributing the coarse grid points within each subdomain.
Optimized transmission conditions stem from a similar idea, namely, to approximate what are called optimal transmission conditions which also leads to convergence of the domain decomposition method in a finite number of iterations. Since these optimal transmission conditions are non-local, in practice one uses local approximations. For RAS we consider here Robin transmission conditions instead of the classical Dirichlet ones, i.e. a well-chosen combination of Dirichlet and Neumann values at subdomain interfaces. A good choice of the Robin coefficient representing the relative weight of Dirichlet and Neumann values permits minimizing the number of iterations, which led to the name Optimized Schwarz Methods. We follow here the method described in [O. Dubois, M.J. Gander, S. Loisel, A. St-Cyr, D.B. Szyld, The Optimized Schwarz Methods with a Coarse Grid Correction, SIAM J. Sci. Comp., vol 34(1), 2012] which only requires modifying the diagonal entries of interface nodes in the subdomain matrices. Again, a good choice of these diagonal entries, for which closed form formulas are available based on the mesh size and the problem parameters, leads to much faster convergence of the associated domain decomposition method than using the standard diagonal entries from RAS.

Our implementation is based on PCASM and, additionally, uses preconditioner composition for the coarse correction (the PCASM is multiplicatively composed with a self-defined PCSHELL implementing the coarse correction) and submatrix modification (PCSetModifySubMatrices) for optimized Robin coefficients. We combine these two improvements and apply them to a 2D Laplace test case up to 16384 cores. We obtain substantially improved computation times with this new optimized 2-levelRAS method which, despite a larger memory footprint, proves to be competitive with the multigrid library HYPRE (with the default options of the PETSc interface to this library).

Consensus Least-squares Reverse Time Migration

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Nowadays, the efficiency of data acquisition technologies provides growing size of seismic data which can improve the imaging of the earth using state-of-the-art reverse time migration (RTM). Least-squares RTM tries to estimate an earth reflectivity image which, via a finite-difference solution to the wave equation, explains all of the reflection gathers in the least-squares sense. In this paper, in order to efficiently solve the regularized least-squares RTM via distributed optimization algorithms, we first reformulate it into a consensus form. Then we solve the resulting consensus RTM efficiently by the Alternating Direction Method of Multipliers (ADMM) algorithm. A main advantage of the new formulation is that the optimization problem is split into separate subproblems, which can be solved in parallel. Specifically, each shot gather is migrated by a node, called worker, to determine the associated image. Then the workers send their local image to another node, called the master, which is responsible for updating the consensus image based on the common image gathers received from the workers. Subsequently, the updated consensus image is distributed back to the workers to drive the new local images into it. This process is iterated until a convergence is achieved.