Numerical Analysis of Coupled and Multi-Physics Problems with Dynamic Interfaces

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1 Overview of the Field

Mathematical models that couple different physical phenomena are ubiquitous in natural and applied sciences. Models coupling elasticity, fluid dynamics and electromagnetism, interfacial and bulk processes are among the most prominent examples. Numerical analysis and simulations of these and other coupled multi-physics problems are crucial for their better understanding, prediction and design. Mathematical analysis and insights are also vital to make progress in these directions.

Many such problems are casted as a system of coupled partial differential equations (PDEs). Sometimes, the PDEs describing different physics can be posed on the same domain, but often various physical processes happen in finitely many disjoint sub-domains separated by evolving interfaces. In addition, the bulk phenomena can be coupled to a process on the interfaces. In such a situation, bulk processes are described by PDEs in sub-domains with solutions glued together by interface conditions and coupled to a mathematical model of the interface dynamics and possibly to a PDE posed on the hyper-surface. One well-known example is the dynamics of two immiscible fluid with soluble surfactants (surface active agents), when the fluid motion in two phases is coupled to the interface evolution as well as to the transport and diffusion of the solute in the bulk phases and along the interface [1]. There are several well-known challenges for numerical analysis and methods development for coupled systems with dynamical interfaces: 1) It is typical that the mathematical analysis of coupled systems is less developed and their mathematical properties are not so well understood, comparing to those of each of the individual component; 2) interface dynamics is defined implicitly as a part of the solution; 3) the interface may undergo topological changes and develop singularities; 4) the bulk solutions may experience the loss of regularity even along smooth interfaces, which makes numerical approximations less accurate or unstable. All these hinder the analysis and development of numerical algorithms for such problems, so that the progress here requires a cumulative effort of applied and computational mathematicians working in a diverse variety of fields and applications.

In addition to the challenges in analysis, solving numerically the fully coupled system at a time can be too computational expensive, while decoupling may produce numerical effects that should be carefully controlled. In order to combat this issue, it is common to consider an iterative scheme where one solves the given PDE in one sub-domain then using the approximation feed a boundary condition to adjoining sub-domains, and iterate this process. The main advantage of doing this is that sophisticated and highly efficient numerical methods have been developed for a single physics problem. For example, consider a fluid–structure interaction problem, which is of great interest in cardiovascular applications [2]. In this problem, in part of the domain there is a fluid (modeled by, say, the Navier-Stokes equations) and the other part a solid model (modeled by equations of elasticity). There are very good and efficient numerical methods for Navier-Stokes and many excellent methods for elasto-dynamics and one takes advantage of this. One of the challenges of using an iterative scheme is the stability of the numerical method. This is especially the case for higher order numerical methods where essentially little progress has been made.

As pointed out above, solutions to coupled problems might have singularities along interfaces as well as the interface itself may develop geometrical singularities and therefore, standard numerical method will behave poorly near the interface. There are several strategies utilized to deal with the loss of accuracy both numerically and at the level of analysis. One is to refine the computational mesh towards the interface and *fit* it to the surface. This, however, is computational expensive for dynamics problems where the interface moves which would require re-meshing at each time step. The second approach is to use a fixed background mesh and modify the numerical method near the interface, for example by building local basis functions on the partition-of-unity [3]. There have been some success in the second approach, however much remains to be done, especially in quantifying geometrical errors, analysing stability and asymptotic behavior of numerical methods.

Coupled and multi-physics problems with propagating interfaces have given rise to very important numerical methods that are widely used. These include, the immersed boundary method [4], the immersed interface methods [5], the level set method [6], eXtended finite element method (XFEM) [7] and cut FEM [8], to name a few. These methods are used for engineering, biological, and physics problems. However, the numerical analysis, i.e. the mathematical foundation of applying these methods, is often lacking and it sometimes takes a long time for a breakthrough idea emerging in computational methods for a particular application to cross boundaries of the field. In many cases people focus on one set of numerical methods or techniques and there lacks discussion among camps.

We brought together different expertise that use different numerical techniques and mathematical analyses. This lead to critical comparison between numerical methods and hopefully lead to new and improved hybrid methods. Without forgetting the applications, we focused mainly on the fundamental mathematical aspects of numerical methods: stability analysis, well-posedness, rigorous error estimates, computational complexity, etc.

The goals of this workshop were as follows:

• Discuss recent advances in the development and mathematical analysis of numerical method for multi-physics problems of interest. All these problems feature propagating interfaces and coupled physical phenomena, possibly happening over different scales.

• Bring together a wide variety of experts to confront some of the challenges that remain in the numerical analysis of interfacial coupled and multi-physics problems.

• Have a critical comparison between different numerical techniques that will lead to better hybrid techniques.

• Focus on foundations of numerical methods for coupled multi-physics problems. Challenge a broader community with mathematical aspects of such problems, which are crucial for the further development of numerical algorithms.

2 Participants

We had an excellent workshop with 40 total participants from North America, Europe and South America. There was a good mix of senior and junior participants. Of all the participants, 4 of them were women. There were 5 graduate student participants. Finally, 11 participants were from Mexico.

Ayuso, Blanca, Universita degli Studi di Bologna
Badia, Santiago , Universitat Politcnica de Catalunya
Balam, Reymundo, Itz CIMAT

Balbas, Jorge California State University-Northridge
Barahona, Igor, Universidad Nacional Autnoma de Mxico
Becker, Roland, Universit de Pau
Boffi, Daniele, University of Pavia
Caballero, Rogelio Oscar, UNAM
Capistrn, Marcos A., CIMAT Guanajuato
Chan, Jesse, Rice University Daz Viera, Martn Alberto, Instituto Mexicano del Petleo
Ern, Alexandre, University Paris-Est
Gastaldi, Lucia, Universit degli Studi di Brescia
Gonzalez Casanova, Pedro, Universidad Nacional Autnoma de Mexico
Guermond, Jean-Luc, Texas A&M University
Guerrero, Zamantha, UNAM
Guzman, Johnny, Brown University
Hao, Wenrui, Penn State University
Hernndez-Dueas, Gerardo, Universidad Nacional Autonoma de Mexico
Li, Zhilin North Carolina State University
Lin, Tao, Virginia Tech
Madureira, Alexandre, Laboratorio Nacional de Computacao Cientifica
Massing, Andre, Umea U.
Mori, Yoichiro, University of Minnesota
Neilan, Michael, University of Pittsburgh
Olshanskiy, Maxim, University of Houston
Owen, Justin Texas A&M University Pea Garca, Jos Alberto , IMATE, UNAM
Peszynska, Malgorzata, Oregon State University
Quezada de Luna, Manuel, U.S. Army Corps of Engineers
Reusken, Arnold, RWTH Aachen University
Rosales Alcantar, Csar Alberto, UNAM
Ruiz-Baier, Ricardo, Oxford U.
Salgado, Abner, U. Tennessee
Sandoval Sols, Mara Luisa, Universidad Autnoma Metropolitana
Sarkis, Marcus, Mathematical Sciences Department - Worcester Polytechnic Institute
Showalter, Ralph E., Oregon State University
Siegel, Michael, New Jersey Institute of Technology Vassilevski, Yuri, Inst. Numerical Mathem RAS Velasco Garca, Ulises, UNAM

3 Presentation Highlights

We had a total of 29 presentations each of which was 40 minutes long. We ended the conference with a two hour discussion where we summarized the talks and open problems were discussed. We received personal feedback from several participants that we list at the end of the report, but here we summarize them.

There were talks in numerous amount of competing numerical methods. This allowed us to compare and led to a nice discussion of pros and cons of different approaches. Among the methods presented were: immersed FEM, hybrid higher order method, discontinuous Galerkin method, Cut-FEM, Level Set method, Genarilzied mass lumping, boundary integral methods, multiscale methods, and immersed interface methods.

We also had several applications and problems : Hele-Shaw equation, Boussinesq equations and atmoshperic modeling, modeling of droplets, multiscale problems, coupling of Navier Stokes and elasticity, to name a few.

Several theoretical PDE questions were also addressed. The Peskin problem which is the basis of the immersed boundary element method was shown to be well posed and regularity was given for Stokes problem with singular sources.

Finally, several numerical thechniques that addressed computational complexity was provided: preconditioners, domain decomposition methods, etc.

4 New Directions and Open Problems

We received personal feedback from several participants that included open problems which are listed at the end of report. Here we give a summary.

Several speakers said that although they have mathematical modesl they would like to address the mathematical well-posedness of the model. Also, several participants mentioned that very small amount of work has been done for interface problems coming from electro-magnetism– They suggested working on this problem. Higher order stable methods for fluid structure interaction problems was listed as an open problem. A few presenters mentioned that they would like to pursue application in biology. Finally, convergence theory of several numerical methods is lacking and is listed as a priority.

5 Individual feedback of participants

Speaker: Tao Lin

Title: A Fixed Mesh Method with Immersed Finite Elements for Solving Interface Inverse Problems

Summary and Highlights:
We consider applying immerse finite elements (IFE) in the shape optimization for solving interface inverse/identification problems. With IFE discretization, the shape optimization is reduce to a constrained optimization problem with the following features:

1. On a fixed mesh, regardless of the location of the interface, the constraint equations in the optimization is an optimal approximation to the PDE constraint system in the shape optimization.

2. On a fixed mesh, regardless of the location of the interface, the cost function in the optimization is an optimal approximation of the cost functional in the shape optimization.

3. The intrinsic dependence of the IFE function on the interface enables us to derive the formula (not an approximation procedure) for the gradient of the cost function in the optimization and this formula can be implemented efficiently within the IFE framework.

The three features listed above collectively distinguish the IFE shape optimization method from those in the literature for solving interface inverse/identification problems.
Outstanding problems and new directions:

1. It was exciting to hear Dr. Yoichiro Mori's report on the local existence and regularity of Peskin's problem for the Stokes flow. It will be interesting to see results for the global existence and regularity.

2. Numerical analysis, both the a-priori and posteriori error estimations for Peskin's problem.

3. Posteriori error estimation for structured/Cartesian mesh methods to solve interface problems and its applications to mesh refinement strategies.

4. Structure/Cartesian mesh methods for more challenging interface problems such as the Maxwell system.

Speaker: Wenrui Hao

Title: Bifurcations arising from a generalized Hele-Shaw problem
Summary and Highlights:

1. A generalized Hele-Shaw problem introduces theoretical and numerical challenges for computing bifurcations.

2. This new model provides a general framework coupling biological networks with porous medium

3. Applications of this new modeling approach to cardiovascular disease also brings multiphysics challenges.

Outstanding problems and new directions:

1. How to develop a robust finite element solver for biological systems?
2. How can we guarantee the solver's robustness as parameters change?

Speaker: Alexander Ern

Title: Hybrid High-Order methods for interface problems
Summary and Highlights:

1. overview on Hybrid High-Order methods: devising and analysis
2. building bridges between hybrid (face-based) methods, notably HHO and HDG
3. applying HHO to interface problems on uniftted meshes
4. cut robustness by polyhedral mesh agglomeration
5. proofs of multiplicative and discrete trace inequalities under general mesh assumptions

Outstanding problems and new directions:

1. unifying viewpoint on hybrid discretization methods for elliptic PDEs and for computational mechanics (including HDG, WG, MHM and others)
2. extend hybrid methods to more complicated interface problems (nonlinear, time-dependent)
3. efficient preconditioners and solvers for hybrid discretization methods

Speaker: Santiago Badia

Title: Unfitted finite element simulations based on cell aggregation

Summary and Highlights:

1. Solve the small cut cell problem for conforming FEM using cell aggregation techniques
2. The method does not introduce additional artiificial diffusion for coercive problems
3. It solves the condition number problem, keeping stability and acuracy
4. Extended to the (Navier-)Stokes problem using mixed FE methods
5. Stable aggregated mixed FEM with minimal pressure stabilization
6. Development of scalable unfitted FE framework, combining octree mesh generation and parallel solvers
7. Applications in additive manufacturing, high-temperature superconductors, and stochastic optimization

Outstanding problems and new directions:

1. Treatment of moving interfaces in time
2. Scalable solvers and large scale simulations with unfitted FE methods
3. Robust methods for practical problems, minimal parameter tunning
4. Minimize artificial diffusion on boundaries/interfaces

5. Efficient numerical integration in unfitted FEM
6. Geometrical handling: how to automatically deal with CAD in embedded frameworks?
7. Automatic implicitization of CAD surfaces
8. High order automatic geometrical approximation with unfitted FEs
9. High order methods for interface-coupled problems in space-time
10. Compatible discretizations

Speaker: Roland Becker

Title:
Summary and Highlights:

1. Comparison of FEM for the high contrast interface problem
2. Alternative Nitsche-type formulations

Outstanding problems and new directions:

1. What is the ultimate low-order FEM for moving interfaces ?
2. Which stabilization/penalization terms are really necessary ?
3. Maximum principle for interface problem
4. Robust a posteriori error estimates
5. Better understanding of conditioning (an estimate of the condition number doesn't seem to me to be sufficient)
6. Simple benchmark problems for FSI (Peskin-problem, Hele-Shaw,...)
7. Optimization, Interface identification

Speaker: Manuel Quezada de Luna

Title: A phase conservative, monolithic level-set method with built-in redistancing
Summary and Highlights:

- Monolithic VOF-like model for level set.
- Phase conservation providing signed distance property with natural representation of the interface.
- Flux correction via diffusion terms penalizing the residual of the Eikonal equation.
- Robust finite element discretization based on a regularized mixed form of the model.
- Use of a single tunable parameter and no need of numerical fixes.
- Efficient quasi-Newton methods for the nonlinear discrete problem.
- Weak coupling with Navier-Stokes solver to solve multiphase incompressible flow.
- Robust for a wide range of benchmarks and applications.

Outstanding problems and new directions

- Instabilities due to weak coupling between fluid and solid solvers; e.g., added mass instability.

- Enhance coupling between fluid and solid solvers via monolithicity, including extra coupling terms and/or post-processing.
- Extending theory and analysis to more realistic applications.
- Need to compare and converge different FSI approaches such as immersed boundary method, shifted boundary method, cut cell methods, extended finite element method, aggregated unfitted finite element method, etc.
- Need on emphasizing more pragmatical concerns such as robustness, scalability, feasibility and simplicity for implementation in existing codes.

Speaker: Malgorzata Peszynska

Title: Phase interface in multi-component mixture
Summary and Highlights:

1. High order accuracy is important for models which we know well and for which we have accurate data that can be used to validate
2. Low order stable algorithms may be sufficient for explorations of models and phenomena for which limited observations/data are available
3. Coupled processes require further novel approaches in analysis, discretization, and solvers since typically their structure is not canonical
4. Problems with interfaces are ubiquitous in applications and rich in challenges but a general framework may not be possible or useful

Speaker: Ralph E. Showalter

Title: A Pseudo-Parabolic PDE for Compaction of a Sedimentary Basin
Summary and Highlights:

1. Compaction is a poromechanical process that combines fluid filtration with deformations containing hysteresis together with elastic or viscoelastic responses in the medium. All of these are present in sedimentary basins at various depths. We showed the viscoelastic component is accurately described by a nonlinear pseudo-parabolic equation that reflects properties of the medium. It remains to
2. model the nonreversible hysteresis damage effects in the medium, and combine all mechanical responses in a common system,
3. identify the ‘interfaces’ that indicate the surfaces delineating these processes, and
4. formulate the free-boundary problem describing the upper surface of the sediment.

Speaker: Gerardo Hernandez-Duenas

Title: Water vapour and rain dynamics in precipitating turbulent convection
Summary and Highlights:

1. A minimal model was presented for precipitating turbulent convection.
2. The model allows for phase changes between water vapour and rain water.
3. The minimal model that we presented uses a Boussinesq approximation, assumes fast auto conversion, fast rain evaporation and neglects ice.
4. The model was tested with simulations of squall lines and scattered convection.

5. The model qualitatively captures observations made in nature and also seen in more comprehensive cloud resolving models, such as propagation of squall lines with tilted profiles, cold pools, and scattered convection.

Outstanding problems and new directions:

1. Global well-posedness of such models.
2. Applications of related models to understanding phenomena such as hurricane embryos.

Speaker: Blanca Ayuso de Dios

Title: ome Simple Preconditioners for Unfitted Nitsche discretizations of interface elliptic problems
Summary and Highlights:

1. simple one level and two level preconditioners for Cut-fem approximation of elliptic high contrast problem
2. analysis of the asymptotic convergence
3. robustness and optimality

Outstanding problems and New Directions:

1. Better understanding on construction (and analysis) of solvers
2. Optimality with respect to polynomial degree of different approaches
3. Common framework for solvers of the different unfitted discretizations
4. Solvers for more general problems (curl-curl, Maxwell, but this requires first understanding the discretization
5. Analysis of AMG in this context...
6. Design of unfitted methods with conservation properties: able to preserve at the discrete level physical properties conserved by the continuous solution. Otherwise design of techniques that can be used to render some of the unfitted methods structure preserving discretizations.
7. Fair comparison of different unfitted techniques on different problems (and applications)?
8. efficient use in time evolving problems?
9. Maxwell & interfaces: discretization etc..
10. Nonlocal problems with interfaces...
11. A-posteriori analysis (this surely could be related to design of solvers)

Speaker: Jesse Chan

Title: Energy-based methods for time-dependent acoustic and elastic wave propagation
Summary and Highlights:

1. "weight-adjusted" mass matrices generalized mass-lumping
2. these approximate weighted mass matrices have explicit low-storage inverses
3. explicit high order error estimates involve the regularity of the weight
4. WADG results in simpler formulations for multi-physics (e.g. acoustic-elastic coupling)

Outstanding problems and new directions

1. Explicit time-domain discretizations:
   - Efficient high performance implementations
   - Preserving stability and high order accuracy
2. Quadrature
3. Analysis of variational crimes or discrete "tricks".

Speaker: Abner Salgado
Title: The Stokes problem under singular forcing Summary and Highlights:

1. Several applications, like active thin structures, immersed interface methods, etc. require to consider the motion of an incompressible flow with a very rough source.
2. We show the well-posedness of the Stokes problem over Lipschitz domains assuming only that the source belongs to a weighted space, and the weight does not have singularities/degeneracies near the boundary.
3. We propose a posteriori error estimators for the Stokes problem with a Dirac delta source and inf–sup stable pairs. We show the reliability and efficiency of these estimators.
4. We propose a posteriori error estimators for the Stokes problem with a Dirac delta source and certain stabilized pairs: $(\mathbf{P}_1, \mathbf{P}_0)$ and $(\mathbf{P}_1, \mathbf{P}_1)$. We show the reliability and efficiency of these estimators.

Outstanding problems and new directions

1. The development of a posteriori error estimators for more other rough sources, like Dirac deltas supported on curves and surfaces.
2. To study the well-posedness of more general fluid models over Lipschitz domains and under singular sources.
3. The numerical analysis of more general fluid models over Lipschitz domains and under singular sources.

Speaker: Yuri Vassilevski
Title: A stable scheme for simulation of incompressible flows in time-dependent domains and hemodynamic applications
Summary and Highlights:

In my talk I presented analysis and numerical study of a monolithic finite element method for the incompressible Navier–Stokes equations coupled to the Saint Venant–Kirchhoff elasticity model. The approach strongly enforces the coupling conditions on the fluid–structure interface and treats both solid and fluid equations in a reference domain accounting for geometric motion through time-dependent coefficients. I presented an energy balance for the fully discrete system and a statement on numerical stability of the proposed finite element method. I demonstrated good performance of the method on several 2D and 3D benchmarks including the pressure impulse propagation test and a recently proposed experimental 3D fluid-structure interaction benchmark problem. In the final part of the talk I presented a reduction of the FSI scheme to the case when the motion of walls is known, applicable to patient-specific simulation of blood flow in human left ventricles. Analysis of the reduced scheme and simulation results were demonstrated.
Outstanding problems and new directions

1. Development of an unified approach for the choice of equation for displacements in fluid domain: the existing solutions are ad hoc.
2. Development of an efficient parallel solver for appearing linear systems.

3. Development of a robust stabilization of the convective term in the Navier-Stokes equations in case of ventricle flow.

Speaker: Michael Siegel

Title: Accurate and efficient boundary integral computations for interfacial flow with surfactant
Summary and Highlights:

1. Accurate and efficient numerical methods were presented for the simulation of the deformation of drops and bubbles in Stokes flow with surfactant. Both insoluble and soluble surfactant were considered.
2. For insoluble surfactant, a new boundary integral (BI) method was presented in which a special quadrature originally developed by Helsing and Ojala is used to retain accuracy for close dropdrop interactions (joint work with Sara Palsson and Anna-Karin Tornberg, KTH).
3. For soluble surfactant, longstanding work and recent results were described on the development of a hybrid or multiscale boundary integral method that resolves a transition layer of bulk soluble surfactant near the interface (with Jacek Wrobel and Michael Booty, NJIT).
4. Large surfactant gradients in the transition layer were resolved by incorporating a separate, singular perturbation analysis of the dynamics in the transition layer into a full numerical solution of the free boundary problem.
5. The boundary integral method was adapted to include flow focussing provided by two transverse, coaxial annular baffles placed symmetrically on either side of a droplet in an imposed extensional flow, as a model of recent experiments.
6. The hybrid method is capable of computing resolved examples of 'tipstreaming,? in which a long thin filament is emitted from the ends of a drop in an imposed extenional flow. Its dependence on parameters such as flow rate and bulk surfactant concentration were investigated and compared with experiments.

Outstanding problems and new directions

1. Development of accurate and efficient FSI methods that include stochastic/Brownian motion which satisfy fluctuation/dissipation theorem.
2. Convergence theory (especially for boundary integral methods).
3. Further development of multiscale methods and application to more complicated problems from multiphysics applications.

Speaker: Alexandre Madureira

Title: Localized Spectral Decomposition (LSD): a robust and efficient finite element method for solving elliptic PDEs
Summary and Highlights:

1. The method is robust with respect to high contrast coefficients
2. it's a true "multiscale method," in the sense that it converges in a quite general setting, i.e., it does not depend of periodicity of the coefficients or other special configurations. It contains interface problems as a particular case.
3. it's embarrassingly parallel, based on two-level meshes
4. the size of the final system is independent of the small scale

Outstanding problems and new directions

1. to investigate dynamic aspects of multiscale problems, and how methods as I described above can accommodate for that. For instance, in dynamic PDEs, coefficients might change with time, and in principle local solutions have to be recomputed. Is there a way to make this efficient?

2. Can multiscale methods like LOD be made as efficient as cutfem for interface problems? Is there a way to find stabilization parameters in cutfem methods in an automatic way? This was done in the 1980's for singular perturbed problems.

Speaker: Zhilin Li

Title: Least Squares Augmented Methods for Fluid and Porous Media Couplings
Summary and Highlights:

1. Fluid and porous media (Stokes/Darcy or Navier-Stokes/Darcy) coupling
2. Literature review on numerical methods on structured meshes
3. Literature review on IFEM, IIM, x-FEM, and augmented methods
4. New methods for solving fluid and porous media coupling using past Poisson solvers.
5. Some new interesting physical phenomena are obtained using the new method.

In summary, the workshop was stimulating. I noticed that the participants were predominately from FEM field. We might have more interesting discussion if we include participants from different fields.

6 Re-activating MexSIAM

Johnny Guzmán, Malgorzata Peszynska (President of SIAM PNW) and Gerardo Hernandez-Duenas had conversations during the workshop to reactivate MexSIAM, the Mexico Section of the Society for Industrial and Applied Mathematics (www.mexsiam.org). MexSIAM was reactivated soon after the workshop and has started activities.

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