# BIRS Workshop 18w5148: Adaptive Numerical Methods for PDEs with Applications

Christopher J. Budd (University of Bath)
Ronald D. Haynes (Memorial University of Newfoundland)
Weizhang Huang (University of Kansas)

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## 1 Overview

Scientific computing is an increasingly important tool in many areas of science and engineering. By simulating models of physical phenomena on a computer we can, for example, gain insight into processes that are difficult or impossible to measure experimentally. Such computations can be used to verify or guide theoretical explorations. Here we are driven by physical solutions which would require prohibitive computational resources if implemented in a naive way. The solutions evolve on disparate space and time scales requiring techniques which self adapt and direct computational resources to the regions of interest.

Adaptive moving mesh methods have received increasing attention from researchers and practitioners over the last two decades. These methods, either used as stand-alone methods or combined with other adaptive mesh methods, are capable of producing meshes of good quality (smoothness and alignment), and meshes which resolve the features of interests in the physical solution with significant increases in accuracy whilst reducing the computational cost. Capitalizing on the recent progress, there is a continuing effort to improve the efficiency of existing methods and to implement these approaches in numerical solvers for application problems of interest.

Loosely speaking, there are three types of adaptive mesh methods, $h$-, $p$-, and $r$-adaptive methods. $h$-adaptive methods achieve adaptivity by adding and deleting mesh points and swapping mesh edges/faces while $p$-adaptive methods do so by adjusting the order of solution approximation over mesh elements. On the other hand, $r$-adaptive methods, also called adaptive moving mesh methods or more simply, moving mesh methods, achieve desired adaptivity by relocating or moving mesh points. The mesh connectivity is kept fixed during mesh movement; nevertheless, the mesh points can be reconnected between time steps or iterations. Adaptive moving mesh methods can be used alone or combined with $h$- and $p$-adaptive methods. It should be pointed out that Lagrangian methods and arbitrary Lagrangian-Eulerian (ALE) methods in computational fluid dynamics are special types of adaptive moving mesh methods. Moreover, mesh smoothing methods such as Laplacian smoothing and optimization-based smoothing methods employed in mesh generation and mesh refinement can be viewed as a type of moving mesh method although their goal is to improve mesh quality.

Whilst $h$-adaptive methods are now mature in their development, the newer $r$-adaptive methods show much promise, and have certain advantages in that they have much less complex data structures, can be easily coupled to legacy codes, they are well suited to problems with moving boundaries and/or Lagrangian structures, and often result in much more regular meshes. However, they have yet to realise their full potential on seriously large problems and need to be mapped effectively to many-core computing technologies.

The time is ripe for a careful appraisal of these methods and to plan for their future development and adoption. This was the aim for this meeting.

# 2 Meeting Particulars

This five day workshop attracted 37 participants which included 10 females and 6 graduate students. The five days included 25 talks of varying length (keynote and contributed talks) as well as an evening whole group brainstorming and planning session.

The meeting saw leading experts in the design and application of $r$-adaptive methods address the following topics:

- The effectiveness and design of mesh movement strategies to adapt to a function (which may be a solution of a PDE) to minimize interpolation/truncation error or satisfy other considerations. Deriving rigorous results to show that this has been achieved.

- The effectiveness and design of mesh movement associated with changes in the physical domain (free or moving boundary problems) or problems with complex boundary conditions.

- Mesh movement for better mesh quality (mesh smoothing, used in mesh refinement and quality improvement).
- Mesh rezoning in ALE methods (Arbitrarily Lagrangian-Eulerian in computational fluid dynamics).
- Coupling mesh movement to the solution of an evolving PDE. In particular effective strategies for dealing with large scale advection dominated problems.
- Preservation of qualitative solution properties (such as conservation laws, geostrophic balance) under mesh movement strategies.
- Mesh movement on manifolds.
- Computing adaptive meshes with global quality effectively on many–core compute technologies.

The brainstorming session included a discussion on the future of the research area and larger research community in adaptive meshing and $r$-refinement. This included discussion about

- The development of effective test problems suitable for a wide variety of adaptive meshes, and a comparison of techniques on large scale application problems.
- A permanent website for the research community to share research papers, computer codes, and meeting announcements.

The central goal of this event was to encourage participants to join their expertise for the mutual benefit of developing, testing, appraising and designing, effective moving mesh methods which can be used on challenging problems in the future.

# 3 Presentation Highlights

The complete list of talks and abstracts are available on the BIRS website. Here we mention a small sample of a few highlights.

Mikhail Shashkov, a senior researcher in the field, gave a talk entitled *Adaptive reconnection-based Arbitrary Lagrangian-Eulerian method*. In this talk he presented a new adaptive reconnection-based Arbitrary Lagrangian Eulerian method. This method includes an explicit Lagrangian phase on arbitrary polygonal meshes in which the solution and positions of grid nodes are updated; a rezoning phase in which a new grid is defined - both number of cells and their locations as well as connectivity (based on using Voronoi tessellation) of the mesh are allowed to change; and a remapping phase in which the Lagrangian solution is transferred onto the new grid.

A post-doc Andrew McRae talked about *Mesh adaptivity on the sphere using optimal transport, and a moving mesh scheme for the nonlinear shallow water equations*. Here the mesh is obtained as the solution of a Monge-Ampere equation, a scalar nonlinear elliptic PDE. This optimal transport approach also generalizes naturally from Euclidean space to manifolds such as the sphere. This method is applied to a finite element shallow water model, as needed in global numerical weather prediction.

In *An adaptive moving mesh method for geometric evolution laws and bulk-surface PDEs*, John Mackenzie considers the adaptive numerical solution of a geometric evolution law where the normal velocity of a curve in two-dimensions is proportional to its local curvature as well as a general non-geometric driving force. An interface tracking approach is used which requires the generation of a moving mesh. He then considers the generation of bulk meshes for the solution of bulk-surface PDEs in time-dependent domains. The moving mesh approach is then applied to a range of problems in computational biology including image segmentation, cell tracking and the modelling of cell migration and chemotaxis.

Graduate student Avary Kolasinski's talk *A surface moving mesh method based on equidistribution and alignment* provides an algorithm to improve the quality of the mesh on a surface using a moving mesh method. She constructs a surface moving mesh method based on mesh equidistribution and alignment conditions. She studies various numerical examples using both the Euclidean metric and a Riemannian metric.

In *Optimal transformation-based adaptive grids*, Paul Zegeling discusses stationary optimal grids for singularly perturbed boundary-value problems. An optimal time-dependent transformation for monotone traveling wave solutions will be proposed. This type of transformation is related to a perturbed method of characteristics. In the final part of the talk, fractional-order differential equations were considered with a discussion of the generation of efficient adaptive grids for these problems.

Jens Lang's talk *Adaptive moving meshes in large eddy simulation for turbulent flows* discussed adaptive moving mesh methods for the Large Eddy Simulation (LES) for turbulent flows. The characteristic length scale of the turbulent fluctuation varies substantially over the computational domain and has to be resolved by an appropriate numerical grid. The monitor function, which is the main ingredient of a moving mesh method, is determined with respect to a quantity of interest (QoI). These QoIs can be physically motivated, like vorticity, turbulent kinetic energy or enstrophy, as well as mathematically motivated, like solution gradient or some adjoint-based error estimator. Results were presented for real-life engineering and meteorological applications.

*A moving mesh finite difference method for non-monotone solutions of non-equilibrium equations in porous media* by Hong Zhang presents a moving mesh finite difference method to solve a modified Buckley Leverett equation with a dynamic capillary pressure term from porous media. The effects of the dynamic capillary coefficient, the infiltrating flux rate and the initial and boundary values are systematically studied using a traveling wave ansatz and efficient numerical methods. The governing equation is discretized with an adaptive moving mesh finite difference method in the space direction and an implicit-explicit method in the time direction. In order to obtain high quality meshes, an adaptive time dependent monitor function with directional control is applied to redistribute the mesh grid in every time step, and a diffusive mechanism is used to smooth the monitor function.

# 4 Meeting Outcome

Moving mesh methods have passed its early development stage (proof-of-concept and algorithm development) and now the time has come for further mathematical justification, rigorous error analysis, development of more efficient and robust methods and implementations, and broader, more realistic, and large scale applications (for example, for problems in atmospherical sciences, computer science, petroleum engineering, aerospace engineering, and biology).

This was the first meeting in many years which brought together senior and up and coming researchers from diverse areas in the field of adaptive numerical methods for partial differential equations. A fantastic exchange of the latest research in the area resulted, as well as crucial planning for the future of the community.