European Trilinos User Group meeting

1 MueLu: The next-generation Trilinos Multigrid Package

Authors Tobias Wiesner (TU München), Ray Tuminaro (Sandia National Laboratory), Jonathan Hu (Sandia National Laboratory), Michael W. Gee (TU München)

Abstract MueLu is the new flexible parallel multigrid package in Trilinos for developing and deploying multigrid algorithms. The framework is designed with a user-friendly front end that also provides an interface to the existing ML package. Prolongator construction methods include smoothed aggregation and Petrov-Galerkin approaches, with plans to add others such as energy minimization. Using the capabilities of Ifpack and Amesos, MueLu includes a standard complement of level smoothers and direct solvers.

The design allows advanced users to customize almost any aspect of the multigrid solver, e.g. introducing specialized transfer operators, applying new smoothers, alternative coarsening algorithms, specialized strength-of-connection measures, and even hybrids of different multigrid algorithms.

In this talk well discuss the main design features. Furthermore we'll illustrate the library usage and demonstrate the flexibility of the MueLu framework with examples.

2 Parallel multilevel incomplete factorization of saddlepoint matrices

Authors Jonas Thies, Fred Wubs (University of Uppsala, Centre for interdisciplinary mathematics)

Abstract We present a Trilinos implementation of a recently developed structure-preserving multilevel preconditioner for a class of saddlepoint problems known as F-matrices. Such matrices arise in the fully coupled solution of the incompressible Navier-Stokes equations on structured meshes. The algorithm is an alternative to the state-of-the-art block preconditioning techniques and has some attractive qualities such as grid-independent convergence, recursiveness and robustness at high Reynolds numbers. The implementation is shown to give good parallel performance for 3D problems with millions of grid cells.

3 Domain decomposition techniques for hyperbolic equations on unstructured grids

Authors Antonio Cervone, Nur Fadel, Luca Formaggia (MOX, Politecnico di Milano)

Abstract The focus of this presentation is set on the numerical implementation of discretized hyperbolic equations on unstructured grids. In this framework, in order to build fluxes for finite volumes or discontinuous Galerkin schemes, information about surrounding values are required. The parallel implementation with the domain decomposition approach creates the need to access information that are defined across the subdomain interface introduced by the partitioning. This work describes a technique to build arbitrary overlapping mappings on the underlying unstructured mesh. These objects, that are based on the parallel MapEpetra object from Trilinos, are then used to develop a parallel solver for interface capturing, based on the level set method, that can track an arbitrary number of species. Some details are also given on the use of this approach to generate physically overlapping mesh partitions that can be used to perform finite element assembly procedures avoiding communication between processes.

4 Preconditioning for Large Scale Micro Finite Element Analyses of 3D Poroelasticity using Trilinos

Authors Peter Arbenz, Erhan Turan

Abstract Poroelasticity investigates the deformation of porous media under the influence of the fluid contained within the body. The classical theory of poroelasticity couples a porous Hookean solid with Darcys law in conjunction with continuity to model the fluid passing through the pores of the solid matrix [3]. Our interest in poroelasticity originates in osteoporosis, a disease that is regarded as a major health problem in developed countries where the risk for an osteoporotic fracture for women above 50 years is about 50%, for men it is about 20%. In this connection, we have developed a solver called ParFE [1] to model linear elastic response of realistic bone structures to exterior forces. The code is highly adapted to voxel-based models generated by CT-scans. It is used by researchers that focus on bone remodelling which investigates the changes on the bone structure exposed to cyclic load.

We present a solver for large scale linear poroelasticity problems considering voxel models on the micro level which will later be used as a tool to analyze bone poroelasticity. The governing equations are discretized using mixed finite elements at which displacements, flux, and pressure are treated primary variables, respectively. The geometry is modeled with equal size hexagonal elements, so-called voxels, in which the approximations are piecewise trilinear (Q1) for displacements and piecewise constant (P0) for the pressure. The flux is approximated by lowest order Raviart-Thomas (RT0) elements.

This mixed finite element discretization leads to a linear system of equations of 3x3 block structure where diagonal blocks are symmetric definite but the system as a whole is symmetric indefinite. There are special iterative (Krylov) methods to solve symmetric indefinite systems, most notably SYMMLQ and MINRES. However, MINRES for example can suffer from loss of orthogonality among the Krylov vectors. Therefore, often GMRES [5] is used instead for solving the linear problem. A Krylov method is only efficient with an appropriate preconditioner. There is a variety of preconditioners available for saddle point problems [2]. In our analysis, we have used two kind of preconditioners: a block diagonal preconditioner and a block triangular preconditioners which utilize the Schur complement on pressue block in particular. An advantage of this idea is that the Schur block can be generated independently by taking advantage of the geometry and the finite element model. Also, this matrix can be approximated efficiently by an AMG V-cycle which is a crucial point in our research.

Our present highly parallel solver, an extension of ParFE [1], relies heavily on the Trilinos framework [6]. Epetra is used to define the matrices and vectors. Belos is selected as the primary iterative solver package. ML is used to employ smoothed aggregation preconditioners on sublocks. IFPACK and Amesos are also considered to compare various adaptions on preconditioning matrix. The solver is tested against benchmark problems on artificial domains and realistic bone structures, all of them composed of voxels. We report on its parallel performance as observed on the Cray XT-5 at the Swiss National Supercomputing Centre (CSCS) and share details of the implemantation.

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5 Ginla: A Trilinos-based solver for the Ginzburg–Landau problem

Authors Nico Schlömer

Abstract The Trilinos-based software *Ginla* for the solution of the nonlinear complex-valued extreme-type-II Ginzburg–Landau equations is presented. As typical for nonlinear equations, the solution landscape is involved and its exploration takes intensive numerical computation. Central algorithmic tools incorporate numerical parameter continuation and a solution strategy for the Jacobian system. Using Trilinos, *Ginla* makes it possible for the first time to compute solutions for actual three-dimensional domains. The software makes direct use of the Trilinos packages LOCA, NOX, Belos, ML, and SEACAS/Stk_mesh and operates on the Epetra stack. Experiences with the individual packages, advantages and downsides of the code, and scalability results will be highlighted."

6 ForTrilinos: Bringing Trilinos to Object-Oriented Fortran Parallel Applications

Authors Karla Morris and Damian Rouson

Abstract This talk will provide a high level description of the infrastructure of the ForTrilinos and CTrilinos packages. These packages support portable, object-oriented (OO) Fortran 2003 interfaces to C++ packages in the Trilinos library and framework [1]. The interfaces are simplified by taking advantage of language features, such as allocatable arrays. ForTrilinos currently offers OO Fortran 2003 interfaces to packages Epetra, AztecOO, and Pliris in Trilinos. Epetra provides distributed matrix and vector storage and basic linear algebra calculations. Pliris provides direct solvers for dense linear systems. AztecOO provides iterative sparse linear solvers. The increase in compiler support for the Fortran 2003 standard allows ForTrilinos to provide Fortran software developers with flexible data structures for parallel applications. These data structures encapsulate the Message Passing Interface (MPI) and circumvent the need for direct calls to MPI, except for startup and shutdown. ForTrilinos enable OO Fortran programmers to write serial code that lower-level abstractions resolve into distributed-memory, parallel implementations [2].

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7 Parallel preconditioners for Saddle-Point problems.

Authors P. Crosetto, S. Deparis, G. Grandperrin, R. Popescu (CMCS - EPFL)

Abstract Approximating a 3-dimensional unsteady flow modeled by the Navier–Stokes equations is very expensive; to lower the time to solution and to address complex problems, a parallel framework as well as specific preconditioners associated to the linearized system are necessary. The important factors to measure parallel performances of a preconditioner are the independence on the number of iterations on the cpu count (scalability of the preconditioner), on the mesh size (optimality), and on the physical parameters (robustness), as well as the strong and weak scalability.

We present a family of preconditioners based on approximate versions of state of the art preconditioners for Navier–Stokes, namely the Pressure-Convection-Diffusion (PCD) preconditioner [6][3], Yosida [5], and SIMPLE [4]. We exploit factorizations of the linearized system where inverses are handle using specific embedded preconditioners. Weak and strong scalability results illustrate this approach using benchmarks relevant to hemodynamics simulations. All the computations are carried out using the open source finite element library LifeV [1] based on Trilinos [2].

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8 Trilinos Progress, Challenges and Future Plans

Authors M. Heroux

Abstract Trilinos has been an open source software project for about nine years. In this presentation we talk about recent progress, current challenges and future plans, focusing especially on efforts for emerging architectures including support for manycore architectures, linear algebra algorithms and fault resilience.