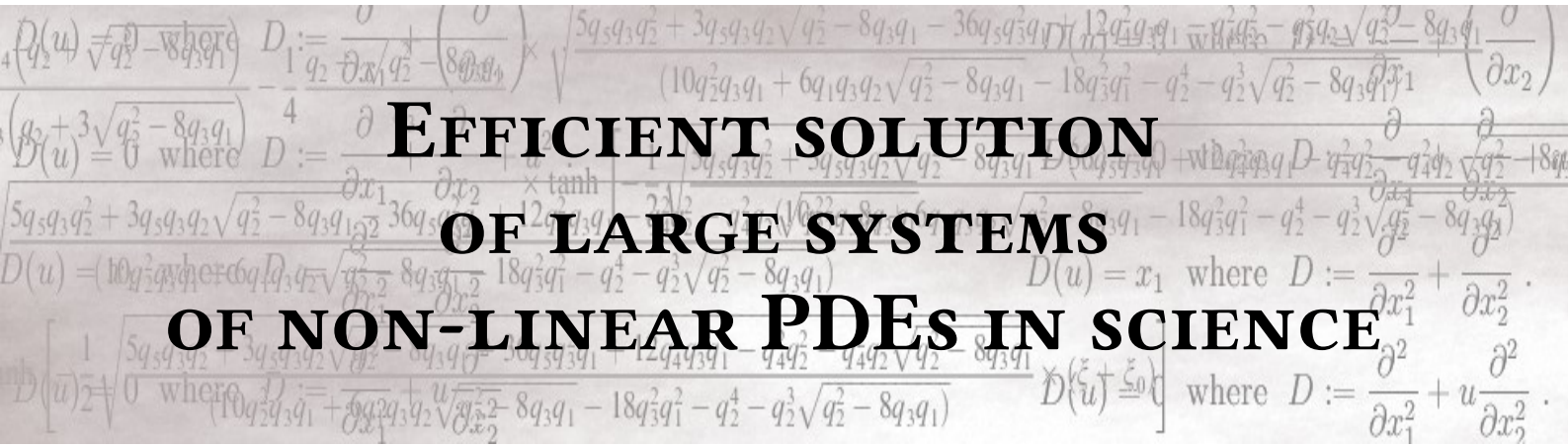


Efficient solution of large systems of non-linear PDEs in science

October 7-9, 2013

Centre Blaise Pascal, ENS Lyon, France

CRA Lyon

CBP Centre Blaise Pascal

FLMSN

Université de Lyon

cnrs

ENS de Lyon

List of participants

1	ARBENZ	Peter	Computer Science Department, ETH Zürich, Switzerland
2	BARAFFE	Isabelle	School of Physics, University of Exeter, UK
3	BERENGUER	Laurent	Université Lyon 1
4	BIRKEN	Philipp	Institut für Mathematik Universität Kassel, Germany
5	CAI	Xiao-Chuan	University of Colorado Boulder, USA
6	CALUGARU	Cerasela	Centre Blaise Pascal, ENS Lyon, France
7	CALUGARU	Dan-Gabriel	Laboratoire de Mécanique des Fluides et d'Acoustique, École Centrale de Lyon, France
8	CHABRIER	Gilles	Centre de Recherche Astrophysique de Lyon, ENS Lyon, France
9	COMMERCON	Benoit	Centre de Recherche Astrophysique de Lyon, ENS Lyon, France
10	CUELLO	Nicolas	Centre de Recherche Astrophysique de Lyon, Observatoire de Lyon, France
11	DE STURLER	Eric	Virginia Tech, USA
12	EDELMANN	Philipp	Max Planck Institute for Astrophysics, Germany
13	FOLINI	Doris	Centre de Recherche Astrophysique de Lyon, ENS Lyon, France
14	GEROUX	Chris	University of Exeter, UK
15	GOFFREY	Tom	University of Exeter, UK
16	HENRY	Daniel	Laboratoire de Mécanique des Fluides et d'Acoustique, École Centrale de Lyon, France
17	INNOCENTI	Maria Elena	Department of Mathematics, KU Leuven, Belgium
18	KÄPPELI	Roger	SAM, Eidgenössische Technische Hochschule Zürich, Switzerland
19	KUPKA	Friedrich	Faculty of Mathematics, University of Vienna, Austria
20	MATSUO	Yoichi	Computer Science Department, ETH Zürich, Switzerland
21	MAY	Dave	Institute of Geophysics, ETH Zürich, Switzerland
22	MELZANI	Mickaël	Centre de Recherche Astrophysique de Lyon, ENS Lyon, France
23	MEYER	Alexandre	Laboratoire d'Informatique en Image et Systèmes d'information, Lyon, France
24	PACULL	Francois	ICJ UMR5208, Polytech Lyon, Université Lyon 1, France
25	POPOV	Mikhail	Centre de Recherche Astrophysique de Lyon, ENS Lyon, France
26	PRATT	Jane	University of Exeter, Astrophysics, UK
27	RUPRECHT	Daniel	Institute of Computational Science, University of Lugano, Switzerland
28	SANCHEZ UMBRIA	Juan	Department of Applied Physics, Universitat Politècnica de Catalunya, Barcelona, Spain
29	SEDLACEK	Jan	Institute of Atmospheric and Climate Science, ETH Zürich, Switzerland
30	TROMEUR-DERVOUT	Damien	ICJ UMR5208, Polytech Lyon, Université Lyon 1, France
31	VAN CRIEKINGEN	Serge	Maison de la Simulation, France
32	VAYTET	Neil	Centre de Recherche Astrophysique de Lyon, ENS Lyon, France
33	VIALLET	Maxime	Max-Planck-Institut für Astrophysik, Germany
34	WALDER	Rolf	Centre de Recherche Astrophysique de Lyon, ENS Lyon, France
35	WINISDOERFFER	Christophe	Centre de Recherche Astrophysique de Lyon, ENS Lyon, France

Efficient solution of large systems of non-linear PDEs in science

October 7-9, 2013

PROGRAM

Monday, October 7, 2013

13:40-17:25	**TUTORIAL ON NEWTON-KRYLOV METHODS**
13:45-13:50	Opening - Rolf Walder
13:50-13:55	The ERC project TOFU - Isabelle Baraffe
13:55-14:40	*Nonlinear Systems of Equations* - Philipp Birken
14:40-15:25	*Newton's Method and Efficient, Robust Variants* - Philipp Birken
15:25-15:55	Coffee Break
15:55-16:40	*Iterative Linear Solvers and Jacobian-Free Newton-Krylov Methods* - Eric de Sturler
16:40-17:25	*Recent Advances* - Eric de Sturler
17:30-18:30	Welcome Apero offered by the TOFU project

Tuesday, October 8, 2013

09:00-09:55	*Scalable multi-level preconditioners for variable viscosity Stokes flow problems arising from geodynamics* - Dave May
09:55-10:40	*Updating Preconditioners for Sequences of Linear Systems* - Eric de Sturler
10:15-11:05	Coffee Break
11:05-11:35	*Using the Jacobian-free Newton-Krylov method to solve the sea-ice momentum equation* - Jan Sedlacek
11:35-12:05	*3-dimensional eigenmodal analysis of electromagnetic structures* - Peter Arbenz
12:05-12:35	*The Multi Level Multi Domain method: a semi-implicit adaptive method for Particle In Cell plasma simulations* - Maria Elena Innocenti
12:35-14:30	Lunch at Brasserie Métropole
14:30-15:15	*A Jacobian-free Newton-Krylov method for time-implicit multidimensional hydrodynamics* - Maxime Viallet
15:15-15:45	*Time-Implicit Hydrodynamics for Gravitational Flows* - Serge Van Criekingen
15:45-16:15	*Well-balanced schemes for the Euler equations with gravitation* - Roger Käppeli
16:15-16:40	Coffee Break
16:40-17:10	*A preconditioned Roe scheme for use in low Mach number hydrodynamical simulations* - Philipp Edelmann
17:10-18:05	*Implicit-Explicit Time Integration Methods for Astrophysical Applications* - Friedrich Kupka
19:00-22:00	Conference Dinner

Wednesday, October 9, 2013

09:00-9:45	*Preconditioners for Discontinuous Galerkin Discretizations of 3D viscous compressible flows* - Philipp Birken
09:45-10:30	*Newton-Krylov based continuation method to study convection in a tilted parallelepiped cavity* - Daniel Henry
10:30-11:00	Coffee Break
11:00-11:55	*Newton-Krylov methods beyond the computation of steady solutions: two applications to Fluid Dynamics problems* - Juan Sanchez Umbria
12:00-14:00	Lunch at Brasserie Métropole
14:00-14:45	*Time-parallel methods for massively parallel solution of PDEs* - Daniel Rupprecht
14:45-15:30	*Newton-Krylov-Schwarz for coupled multi-physics problems* - Xiao-Chuan Cai
15:30-15:35	Closing Remarks - Rolf Walder

Table of Contents

Scalable multi-level preconditioners for variable viscosity Stokes flow problems arising from geodynamics

Dave May [1]
[1] Institute of Geophysics, ETH Zurich, Switzerland
dave.may@erdw.ethz.ch

Here I describe a numerical method suitable for studying non-linear, large deformation processes in crustal and lithospheric dynamics. The method utilizes a hybrid spatial discretisation which consists of mixed finite elements for the non-linear Stokes flow problem, coupled to a Lagrangian marker based discretisation to represent the material properties (viscosity and density). This approach is akin to the classical Marker-And-Cell (MAC) scheme of Harlow and the subsequently developed Material Point Method (MPM) of Sulsky and co-workers. The geometric flexibility and ease of modelling large deformation processes afforded by such mesh-particle methods has been exploited by the geodynamics dynamics community over the last 15 years.

The strength of the Stokes preconditioner fundamentally controls the scientific throughput achievable and represents the largest bottleneck in the development of our understanding of geodynamic processes.

The possibility to develop a "cheap" and efficient preconditioning methodology which is suitable for the mixed Q2-P1 element is explored here. I describe a flexible strategy, which aims to address the Stokes preconditioning issue using an upper block triangular preconditioner, together with a geometric multi-grid preconditioner for the viscous block. The key to the approach is to utilize algorithms and data-structures that exploit current multi-core hardware and avoid the need for excessive global reductions. In order to develop a scalable method, special consideration is given to; the definition of the coarse grid operator, the smoother and the coarse grid solver.

The performance characteristics of this hybrid matrix-free / partially assembled multi-level preconditioning strategy is examined. The robustness of the preconditioner with respect to the viscosity contrast and the topology of the viscosity field, together with the parallel scalability is demonstrated.

Preconditioners for Sequences of Linear Systems

Eric de Sturler [1]
[1] Virginia Polytechnic Institute and State University Blacksburg, VA 24061-0002 - United States

Computing good preconditioners is an important but expensive component of many simulations Therefore, it makes sense to update preconditioners rather than compute them from scratch for sequences of linear systems. This is particularly relevant for problems where we may not have the matrix available directly (matrix-free problems).

We consider several classes of problems and several techniques such as updating factorizations, low rank updates to preconditioners, and updating preconditioners for dynamically adapted meshes Finally, we focus on an interesting approach that can be combined with any type of preconditioner For a sequence of linear systems and a preconditioner for the initial system, we compute a sequence of sparse matrices as cheap maps from each matrix to either the initial matrix or the previous matrix Combined with the initial preconditioner (and possibly previous maps) this gives an effective preconditioner for each matrix at low cost.

Using the Jacobian-free Newton-Krylov method to solve the sea-ice momentum equation

Jan Sedlacek [1]
[1] Eidgenössische Technische Hochschule Zürich, Switzerland

Sea ice, with its insulating properties, plays an important role in the exchange of heat, humidity and momentum in the high latitudes. A good description of the motion of the sea ice is therefore of crucial importance, as sea-ice motion is responsible for the formation of divergence (leads) and convergence zones in the ice pack, which change its insulating properties. The sea-ice momentum equation is highly non-linear because of water drag and the rheology (the relationship between applied stresses and resulting deformations). As climate models move towards higher resolution computational cost plays an increasingly crucial role. I will present our approach for implementing the Jacobian-free Newton-Krylov method as a new solver sea-ice momentum equation and will also highlight difficulties we encountered and address the question on convergence criteria.

3-dimensional eigenmodal analysis of electromagnetic structures

P. Arbenz [1], H. Guo [1] & Y. Matsuo [1]
[1] ETH Zürich, Computer Science Department, Switzerland
arbenz@inf.ethz.ch

The design of Radio Frequency (RF) structures is a complex optimization process. RF structures are elements in which charged particle are accelerated by an oscillating electric field which is obtained by exciting the proper eigenmode of the accelerator cavity. The shape of the eigenmodes as well as their frequencies are determined by the shape of the cavity. Frequencies and eigenmodes are determined by the time-harmonic Maxwell equations.

Our solver Femaxx generally discretizes the time-harmonic Maxwell Equations with the finite element method (FEM) in 3-dimensional space on unstructured tetrahedral grids, in order to model complicated curved geometry. The code is parallelized and optimized for distributed memory parallel computing architectures.

We discuss our approaches for solving the time-harmonic Maxwell equations when there is loss. Femaxx implements the Jacobi-Davidson QZ (JDQZ) method, for solving linear or quadratic eigenvalue problems. The latter includes electromagnetic loss mechanisms in the model.

Femaxx also implements a nonlinear Jacobi-Davidson (NLJD) method. Using a fully iterative scheme of NLJD eigensolvers, we analyze plasmonic nanostructures, fully considering the dispersive dielectric properties of metals in the optical region of the electromagnetic spectrum.

We will in particular discuss our usage of the Trilinos framework.

The Multi Level Multi Domain (MLMD) method: a semi-implicit adaptive algorithm for Particle In Cell plasma simulations

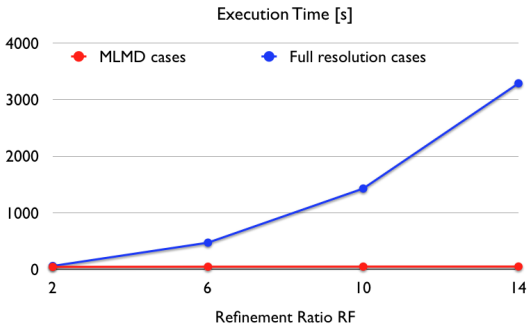
M.E. Innocenti[1], A. Beck[2], S. Markidis[3], G. Lapenta[1]

[1] *KU Leuven, Leuven, Belgium*

[2] *Laboratoire Leprince-Ringuet, Ecole Polytechnique, CNRS-IN2P3, France*

[3] *HPCViz Department, KTH Royal Institute of Technology, Stockholm, Sweden*

The computational effort required by Particle In Cell (PIC) space physics simulations demands the use of increasingly sophisticated numerical methods, since the strict stability constraints of explicit PIC simulations make them very demanding even for the current supercomputing capabilities.



The community has so far tackled this issue in the following ways. Either fully implicit (Chen et al., 2011; Markidis and Lapenta, 2011) / semi implicit (Vu and Brackbill, 1992; Lapenta et al., 2006; Cohen et al., 1989) methods are used to bypass the strict stability constraints of explicit PIC codes or Adaptive Mesh Refinement (AMR) techniques (Vay et al., 2004; Fujimoto and Sydora, 2008) are employed to change locally the simulation resolution. This saves computational resources if only a portion of the domain needs to be resolved with the highest resolution. To the authors' knowledge, however, no code in use combines the benefits of implicit methods and adaptive techniques.

Innocenti et al. (2013) and Beck et al. (2013) have proposed for the first time an adaptive technique which uses as baseline algorithm the Implicit Moment Method (IMM) (Vu and Brackbill, 1992; Lapenta et al., 2006). The use of the IMM allows to taylor the resolution used in each simulated level to the physical scales of interest, without being constrained to resolve the Debye length and the inverse electron plasma frequency on each level for stability reasons, as in explicit AMR codes. As a consequence, very high Refinement Ratios RF (i.e., the ratio in resolution between the levels) are achievable.

The method is named Multi Level Multi Domain (MLMD) to highlight some critical differences with respect to the standard AMR implementations. A major difference is that all the *levels* are simulated as complete *domains*: both fields and particles are simulated also in the areas of grid overlap. This allows the different levels to evolve according to the local dynamics and achieve optimal level interlocking.

The MLMD algorithm is demonstrated by simulating magnetic reconnection (Biskamp, 2005) problems with very high Refinement Ratios between the simulated levels, up to $RF = 12$ per simulated dimension.

The figure illustrates the kind of computational savings registered with the MLMD method. The execution times of two level 2D MLMD simulations with increasing Refinement Ratios RFs between the levels (red line) are compared with the execution times of "standard" simulations performed using the same resolution of the refined level on the entire domain (blue line). As evident, astonishing execution time savings are obtained if only a fraction $1/RF^2$ of the entire domain needs increased resolution.

Beck, A., Innocenti, M., Lapenta, G., and Markidis, S. (2013). Multi-level multi-domain algorithm implementation for two-dimensional multiscale particle in cell simulations. submitted.

Biskamp, D. (2005). *Magnetic reconnection in plasmas*, volume 3. Cambridge University Press.

Chen, G., Chacón, L., and Barnes, D. C. (2011). *Journal of Computational Physics*, 230(18):7018–7036.

Cohen, B. I., Langdon, A., Hewett, D. W., and Procassini, R. J. (1989). *Journal of Computational Physics*, 81(1):151 – 168.

Fujimoto, K. and Sydora, R. D. (2008). *Computer Physics Communications*, 178:915–923.

Innocenti, M., Lapenta, G., Markidis, S., Beck, A., and Vapirev, A. (2013). *Journal of Computational Physics*, 238(0):115 – 140.

Lapenta, G., Brackbill, J., and Ricci, P. (2006). *Physics of plasmas*, 13:055904.

Markidis, S. and Lapenta, G. (2011). *Journal of Computational Physics*, 230(18):7037 – 7052.

Vay, J., Colella, P., Friedman, A., Grote, D. P., McCorquodale, P., and Serafini, D. B. (2004). *Computer Physics Communications*, 164:297–305.

Vu, H. and Brackbill, J. (1992). *Computer physics communications*, 69(2):253–276.

A Jacobian-Free Newton-Krylov method for time-implicit multidimensional hydrodynamics

Maxime Viallet [1],
[1] Max-Planck-Institut für Astrophysik, Garching, Germany

I will present a Jacobian-Free Newton-Krylov method for time-implicit hydrodynamics. I will show that the key ingredient of such a solver is the preconditioner, which has to deal with stiffness arising from fast sound waves. I will present our current implementation of a preconditioning technics known as "Physics-Based Preconditioning", which, unlike algebraic preconditioning, aims at introducing physical properties of the system within the preconditioner itself.

Time-Implicit Hydrodynamics for Gravitational Flows

S. Van Criekingen [1], M. Szydlarski [2],
B. Braconnier [3], J. Vides [1], E. Audit [1],
[1] Maison de la Simulation, Gif-sur-Yvette, France,
[2] University of Oslo, Institute of Theoretical Astrophysics, Norway,
[3] IFP-Energie Nouvelles, Rueil-Malmaison, France.

Within the framework of the 3D hydrodynamical code HERACLES [1] simulating astrophysical fluid flows, we consider the Euler-Poisson model, i.e., the Euler equations supplemented by gravitational effects. We derive a time-implicit resolution scheme from the explicit one developed by Vides et al. [2]. This requires computing a Jacobian, which is done symbolically using the automatic differentiation tool TAPENADE [3] developed at INRIA. The resulting sparse linear system is solved using the PETSc [4] library. We present parallel numerical results for the Rayleigh-Taylor instability obtained on up to eight thousand CPU cores.

References

[1] E. Audit et al. http://irfu.cea.fr/Projets/Site heracles/index.html.
[2] J. Vides, B. Braconnier, E. Audit, C. Berthon, and B. Nkonga. A Godunov-Type Solver for the Numerical Approximation of Gravitational Flows. Communications in Computational Physics, 15(1):46–75, 2014.
[3] Inria Tropics team. http://www-sop.inria.fr/tropics/tapenade.html.
[4] Satish Balay, Jed Brown, Kris Buschelman, William D. Gropp, Dinesh Kaushik, Matthew G. Knepley, Lois Curfman McInnes, Barry F. Smith, and Hong Zhang. http://www.mcs.anl.gov/petsc.

Well-balanced schemes for the Euler equations with gravitation

Roger Käppeli [1]
[1] Seminar for Applied Mathematics, ETH Zürich, Switzerland

Conservation laws with source terms, i.e. balance laws, allow steady state solutions where the flux divergence is exactly balanced by the source term. Standard high-resolution finite volume schemes do not preserve a discrete version of this balance and generate spurious waves that can obscure waves of interest. The main reason for the failure of standard schemes to preserve this equilibrium relies in the fact that it cannot be represented by simple polynomial functions commonly used in the reconstruction step. Therefore, standard reconstruction techniques lead to non-zero truncation errors inducing spurious waves. Schemes that preserve exactly some discrete version of this equilibrium are termed as well-balanced.

In this talk we consider the Euler equations with gravitation. An interesting class of steady states are the hydrostatic ones, where the pressure gradient exactly balances the gravitational force. This type of equilibrium arises for example in the study of atmospheric phenomena that are essential in numerical weather prediction and in climate modeling as well as in a wide variety of contexts in astrophysics such as modeling solar climate or simulating supernova explosions.

We will report on our newly developed well-balanced high-order finite volume schemes to approximate the Euler equations with gravitation. The schemes preserve discrete equilibria, corresponding to a large class of physically stable hydrostatic steady states. Based on a novel local hydrostatic reconstruction, the derived schemes are well-balanced for any consistent numerical flux for the Euler equations. The form of the hydrostatic reconstruction is both very simple and computationally efficient as it requires no analytical or numerical integration.
Moreover, as required by many interesting astrophysical scenarios, the schemes are applicable beyond the ideal gas law. Both first- and second-order accurate versions of the schemes and their extension to multi-dimensional equilibria are presented. Several numerical experiments demonstrating the superior performance of the well-balanced schemes, as compared to standard finite volume schemes, are also presented.
We will especially emphasize astrophysically relevant applications.

A preconditioned Roe scheme for use in low Mach number hydrodynamical simulations

Fabian Miczek[1] , Friedrich Roepke[2] , Philipp Edelmann[1]
[1] Max Planck Institute for Astrophysics (MPA)
Karl-Schwarzschild-Str. 1 85741 Garching bei München - Germany
[2] Universität Würzburg
Campus Hubland Nord Emil-Fischer-Str. 31 97074 Würzburg - Germany

Finite-volume, Riemann-solver-based methods are among the standard methods for the simulation of hydrodynamical flows. While they perform very well in the high Mach number regime, many of them suffer from excessive numerical dissipation at low Mach numbers. Several modified sets of PDEs exist for simulations in this regime. However, in the intermediate regime, in which compressible effects are non-negligible, the original equations have to be solved. We present a new flux preconditioning matrix for Roe schemes solving the compressible Euler equations. It greatly reduces the numerical dissipation and makes it independent of the Mach number. Together with implicit time stepping, this allows us to efficiently simulate low Mach number flows without neglecting compressible effects. To solve the non-linear equations we use the Newton-Raphson method; for the linear system we use a range of Krylov methods together with different preconditioners. We will show some benchmarks of the different solvers.

Implicit-Explicit Time Integration Methods for Astrophysical Applications

Friedrich Kupka [1], Natalie Happenhofer [1], Hannes Grimm-Strele [1] & Herbert Muthsam [1]
[1] Faculty of Mathematics, University of Vienna, Austria

Astrophysical problems are very often described by non-linear, dynamical equations which model processes operating on vastly different spatial and temporal scales. In particular, for the physics of stars and planets the hydrodynamical equations and various extensions thereof can often be used to accurately model the main properties of these physical systems. From a mathematical point of view this leads to quasi-linear partial differential equations of mixed type. Numerical schemes for their solution thus have to be constructed having different classes of equations (hyperbolic, parabolic, and even elliptic) in mind. Weighted essentially non-oscillatory methods are a powerful approach to discretize the advection and pressure gradient terms in these equations. However, the sound waves introduced through the pressure gradient terms may operate on much shorter time scales than the actual advection which takes place in an astrophysical flow and stiff terms due to diffusion or radiative transfer may also impose unwanted, strict limits to time steps achievable by explicit time integration methods. Thus, sophisticated methods are required which can efficiently integrate the resulting systems of equations in time. In this presentation I will discuss new advances made by constructing strong stability presering, implicit-explicit Runge Kutta methods as well as improved versions of a further (time-) operator splitting method developed to deal with pressure gradient terms. The motivation behind contructing these methods will be explained as well as some of their underlying theory, followed by applications of them to astrophysical problems.

Preconditioners for Discontinuous Galerkin Discretizations of 3D viscous compressible flows

Philipp Birken [1], Mark Haas [2], Claus-Dieter Munz [3]
[1] University of Kassel (Supported by the DFG via SFB-TRR 30)
Heinrich-Plett-Str. 40, D-34132 Kassel
birken@mathematik.uni-kassel.de

[2] Robert Bosch GmbH
Postfach 30 02 40, D-70442 Stuttgart
mark.haas@de.bosch.com

[3] University of Stuttgart
Pfaffenwaldring 21, D-70550 Stuttgart
munz@iag.uni-stuttgart.de

Keywords: Discontinuous Galerkin, Navier-Stokes equations, implicit time integration, preconditioning, JFNK

We consider the time dependent three dimensional compressible Navier-Stokes equations and their discretization using discontinuous Galerkin (DG) methods. For wall bounded flows, the boundary layer leads to extremely fine cells, meaning that the use of implicit time integration scheme becomes attractive. Here, we use ESDIRK and Rosenbrock methods, where the appearing linear and nonlinear equation systems are solved using right preconditioned Jacobian-Free Newton-Krylov schemes [5]. As a baseline scheme, these are compared to standard explicit Runge-Kutta schemes and to a type of predictor-corrector schemes that allows local time stepping for DG methods [3].

For implicit schemes, the core difficulty is to find a preconditioner for the block systems that is efficient and uses as little storage as possible, since for DG methods, the size of the blocks is much larger than for finite volume schemes. Furthermore, it should perform well in parallel. The DG method we consider is the polymorphic modal-nodal scheme of Gassner et. al., which uses a modal basis for the representation of the solution [4]. Thus, we suggest the ROBO-SGS preconditioner [1], an SGS method using reduced order offdiagonal blocks, which we find to be significantly better than ILU or the multilevel ILU of Persson et. al. [6]. These reduced blocks can be obtained in a straight forward manner due to the hierarchical basis.

Furthermore, the choice of tolerances in the adaptive time integration scheme, the Newton method and GMRES is an important point. Using embedded error estimators and inexact Newton schemes, where the tolerances are given by the strategy of Eisenstat and Walker [2], we obtain an efficient and accurate time integration scheme that has a good strong parallel scaling. This will be demonstrated by corresponding numerical results.

References

[1] P. Birken, G. Gassner, M. Haas, and C.-D. Munz. Preconditioning for modal discontinuous Galerkin methods for unsteady 3D Navier-Stokes equations. J. Comp. Phys. 11/17
[2] S. C. Eisenstat and H. F. Walker. Choosing the forcing terms in an inexact newton method. SIAM J. Sci. Comput., 17(1):16–32, 1996.
[3] G. Gassner, M. Dumbser, F. Hindenlang, and C.-D. Munz. Explicit one-step time discretizations for discontinuous Galerkin and finite volume schemes based on local predictors. J. Comp. Phys., 230(11):4232–4247, 2011.
[4] G. J. Gassner, F. Lörcher, C.-D. Munz, and J. S. Hesthaven. Polymorphic nodal elements and their application in discontinuous Galerkin methods. J. Comp. Phys., 228(5):1573–1590, 2009.
[5] D. A. Knoll and D. E. Keyes. Jacobian-free Newton-Krylov methods: a survey of approaches and applications. J. Comp. Phys., 193:357–397, 2004.
[6] P.-O. Persson and J. Peraire. Newton-GMRES Preconditioning for Discontinuous Galerkin discretizations of the Navier-Stokes equations. SIAM J. Sci. Comp., 30:2709–2733, 2008.

Newton-Krylov based continuation method to study convection in a tilted parallelepiped cavity

D. Henry [1], H. Ben Hadid [1] and J.F. Torres[1, 2]
[1] Laboratoire de Mécanique des Fluides et d'Acoustique, CNRS/Université de Lyon,
Ecole Centrale de Lyon/Université Lyon 1/INSA de Lyon,
ECL, 36 avenue Guy de Collongue, 69134 Ecully Cedex, France.
[2] Graduate School of Engineering, Tohoku University,
6-6-04, Aramaki Aza Aoba Aoba-ku, Sendai, Miyagi 980-8579, Japan

A continuation method developed from a three-dimensional spectral finite element code is used to study natural convection in a tilted parallelepiped cavity. This continuation method allows the calculation of solution branches, the stability analysis of the solutions along these branches, the detection and precise direct calculation of the bifurcation points, and the jump to newly detected stable or unstable branches, all this being managed by a simple continuation algorithm. The non-linear problems appearing at the different steps (calculation of the solutions, calculation of the bifurcation points) are solved with Newton-Krylov methods based on the linear iterative solver GMRES. After presentation of all these methods and of their efficiency, we will show the results obtained in the study of natural convection in a tilted parallelepiped cavity. The cavity has its length equal to two times the side of its square cross-section and it contains a fluid with a Prandtl number Pr = 1. A detailed bifurcation diagram is first obtained in the case without inclination in order to get the sequence of the different branches of solutions and determine the stable solutions. The focus is then put on the stable solutions in the inclined cavity, when the tilt occurs around the longer axis of the cavity. The subtle changes induced by the tilt on the convective system are clarified. Three different stable solutions are obtained and characterized: the longitudinal roll L– solution (with the same sense of rotation as the inclination angle), the longitudinal roll L+ solution (with a sense of rotation opposite to the inclination angle), and the oblique roll O± solutions (corresponding to transverse roll solutions perturbed by the longitudinal flow induced by the tilt). The domain of existence of these stable solutions is eventually obtained and described in the Rayleigh number-inclination parameter space.

Newton-Krylov methods beyond the computation of steady solutions: two applications to Fluid Dynamics problems

Juan Sanchez Umbria [1], Marta Net [1], Ferran Garcia [1],
[1] Departament de Física Aplicada, Universitat Politècnica de Catalunya, Barcelona, Spain.

The computation by continuation methods of steady solutions of large-scale dynamical systems (ODE/DAE), obtained by discretizing systems of elliptic and/or parabolic PDEs, is a common tool used by researchers in Nonlinear Elasticity and Fluid Mechanics since the late seventies. The efficient computation of other invariant objects by other means than just time evolution is very recent. In the first part of the talk, algorithms based on Newton-Krylov techniques for computing fixed points, periodic orbits, and invariant tori will be presented. Some results of the application of these methods to the thermal convection of a binary fluid mixture in a rectangular two-dimensional box will be shown In the second part the results of the application of Newton-Krylov methods for the computation of travelling waves appearing in the thermal convection of a pure fluid contained in a spherical shell with differential heating are studied. They are computed as steady solutions of a system for the waves, in the frame of reference of the spheres. In this case the special block-tridiagonal structure of the linear part of the equations provides a preconditioner, which allows an efficient calculation. Their stability is also studied, and the secondary bifurcations to modulated waves are detected.

Time-parallel methods for massively parallel solution of PDEs

D. Ruprecht[†], R. Speck[*†], R. Krause[†],
[†]Institute of Computational Science, Università della Svizzera italiana, Switzerland.
[*]Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany.

I. Overview

Todays fastest supercomputers already feature more than a million cores and this number is expected to rise beyond 100 million over the next decade. Because at the same time frequencies of individual processors remain constant or even decrease for reasons of efficiency, developers are increasingly confronted with the fact that accelerating numerical (but also other) codes *necessarily requires to exploit concurrency*. This, in turn, means that concurrency is more and more becoming a critical property of numerical algorithms. To this effect, methods for solving initial value problems that provide concurrency in the temporal direction have been shown to be an effective way to increase the degree of parallelism in the solution of time-dependent PDEs. Several such "time-parallel" methods exist, ranging from the very early interpolation-based scheme in [1] over the parabolic multi-grid method [2] to, more recently, the Parareal algorithm [3] and the "parallel full approximation scheme in space and time" (PFASST) [4]. The talk will focus on both Parareal and PFASST, discuss some of their critical mathematical properties and present benchmarks of the performance of these methods for large-scale parallel solutions of time-dependent PDEs. A very brief summary of the key aspects including multiple references is given below.

II. Parareal

Parareal is at present probably the most popular time-parallel method, as it allows to use basically arbitrary one-step methods within the Parareal iteration. Denoting an accurate but computationally expensive method by $\mathcal{F}$ and a coarse but computationally cheap method by $\mathcal{G}$, Parareal replaces the straightforward serial time-stepping procedure $y_{n+1} = \mathcal{F}(y_n)$, $n = 0, \dots N-1$ by an iteration

$$y_{n+1}^{k+1} = \mathcal{G}(y_n^{k+1}) + \mathcal{F}(y_n^k) - \mathcal{G}(y_n^k), \;\; k = 0, \dots, N_{\text{it}}. \qquad (1)$$

The key here is that once the values y_n^k from the previous iteration are known, the computationally expensive computation of $\mathcal{F}(y_n^k)$ for $n = 0, \dots, N-1$ can be done in parallel on N processors, followed by a serial but cheap correction in which $\mathcal{G}(y_n^{k+1})$ is evaluated and y_{n+1}^{k+1} computed. A detailed discussion of the algorithm plus many additional references can be found e.g. in [5], a detailed mathematical analysis is conducted in [6]. Its speedup using N processors and performing N_{it} iterations can by design not be optimal and is restricted by two competing bounds

$$s(N) \leq \min \left\{ \frac{N}{N_{\text{it}}}, \frac{\text{Runtime } \mathcal{G}}{\text{Runtime } \mathcal{F}} \right\}. \qquad (2)$$

Nevertheless, Parareal can provide additional speedup for the solution of time-dependent problems after spatial parallelization is saturated.

III. PFASST

The PFASST method has been introduced in [4]. It is based on "spectral deferred correction" (SDC) methods [7], an iterative approach for computing collocation solutions. PFASST employs a hierarchy of space-time levels on which iterations of SDC (so-called "sweeps") are performed. These levels are coupled, as in nonlinear multi-grid methods, by an FAS-correction that allows the solution on the coarser levels to converge up to an accuracy determined by the discretization on the finest level. PFASST can also be interpreted as a time-parallel version of a multi-level spectral deferred correction method (MLSDC) [8]. By not solving the fine-level problem to full accuracy but only performing SDC sweeps, PFASST has a significantly improved speedup bound compared to Parareal. Ideal speedup, however, is also not obtainable. The capability of PFASST to be used in parallel simulations on $\mathcal{O}(100k)$ cores has been demonstrated for different scenarios. In [9], it is shown that PFASST can accelerate a particle-based Navier-Stokes solver beyond the saturation point of the underlying spatial parallelization of a Barnes-Hut tree-code [10]. Scaling of PFASST combined with a mesh-based discretization and a parallel multi-grid (PMG) as space-parallel solver for implicit time-stepping is studied in [11] and the impact of using spatial coarsening strategies in large-scale parallel simulations is discussed. Finally, the study is extended in [12], where scaling results of PFASST+PMG on up to all 448K cores of the IBM Blue Gene/Q JUQUEEN at Jülich Supercomputing Centre are reported.

References

[1] J. Nievergelt, "Parallel methods for integrating ordinary differential equations," *Commun. ACM*, vol. 7, no. 12, pp. 731–733, 1964. [Online]. Available: http://dx.doi.org/10.1145/355588.365137

[2] W. Hackbusch, "Parabolic multi-grid methods," *Computing Methods in Applied Sciences and Engineering, VI*, pp. 189–197, 1984. [Online]. Available: http://dl.acm.org/citation.cfm?id=4673.4714

[3] J.-L. Lions, Y. Maday, and G. Turinici, "A "parareal" in time discretization of PDE's," *Comptes Rendus de l'Académie des Sciences - Series I - Mathematics*, vol. 332, pp. 661–668, 2001. [Online]. Available: http://dx.doi.org/10.1016/S0764-4442(00)01793-6

[4] M. Emmett and M. L. Minion, "Toward an efficient parallel in time method for partial differential equations," *Communications in Applied Mathematics and Computational Science*, vol. 7, pp. 105–132, 2012. [Online]. Available: http://dx.doi.org/10.2140/camcos.2012.7.105

[5] D. Ruprecht and R. Krause, "Explicit parallel-in-time integration of a linear acoustic-advection system," *Computers & Fluids*, vol. 59, no. 0, pp. 72 – 83, 2012. [Online]. Available: http://dx.doi.org/10.1016/j.compfluid.2012.02.015

[6] M. J. Gander and S. Vandewalle, "Analysis of the parareal time-parallel time-integration method," *SIAM Journal on Scientific Computing*, vol. 29, no. 2, pp. 556–578, 2007. [Online]. Available: http://dx.doi.org/10.1137/05064607X

[7] A. Dutt, L. Greengard, and V. Rokhlin, "Spectral deferred correction methods for ordinary differential equations," *BIT Numerical Mathematics*, vol. 40, no. 2, pp. 241–266, 2000. [Online]. Available: http://dx.doi.org/10.1023/A:1022338906936

[8] R. Speck, D. Ruprecht, M. Emmett, M. Minion, M. Bolten, and R. Krause, "A multi-level spectral deferred correction method," 2013, arXiv:1307.1312 [math.NA]. [Online]. Available: http://arxiv.org/abs/1307.1312

[9] R. Speck, D. Ruprecht, R. Krause, M. Emmett, M. Minion, M. Winkel, and P. Gibbon, "A massively space-time parallel N-body solver," in *Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis*, ser. SC '12. Los Alamitos, CA, USA: IEEE Computer Society Press, 2012, pp. 92:1–92:11. [Online]. Available: http://dx.doi.org/10.1109/SC.2012.6

[10] M. Winkel, R. Speck, H. Hübner, L. Arnold, R. Krause, and P. Gibbon, "A massively parallel, multi-disciplinary Barnes-Hut tree code for extreme-scale N-body simulations," *Computer Physics Communications*, vol. 183, no. 4, pp. 880 – 889, 2012. [Online]. Available: http://dx.doi.org/10.1016/j.cpc.2011.12.013

[11] R. Speck, D. Ruprecht, M. Emmett, M. Bolten, and R. Krause, "A space-time parallel solver for the three-dimensional heat equation," 2013, arXiv:1307.7867 [cs.NA]. [Online]. Available: http://arxiv.org/abs/1307.7867

[12] D. Ruprecht, R. Speck, M. Emmett, M. Bolten, and R. Krause, "Extreme-scale space-time parallelism," 2013, poster, accepted for SC'13.

Workshop "Efficient solution of large systems of non-linear PDEs in science"
Lyon, France, October 7–9, 2013.

Newton-Krylov-Schwarz for coupled multi-physics problems

Xiao-Chuan Cai [1]
[1] University of Colorado Boulder, United States

Newton-Krylov-Schwarz is a general purpose parallel solution method for solving system of algebraic equations arising from the discretization of nonlinear partial differential equations. In a Newton-Krylov algorithm, the nonlinear system is solved by an inexact Newton method, in which the Jacobian systems are solved with a preconditioned Krylov subspace method. The success of the overall approach depends heavily on what preconditioner is used, and the selection of the preconditioner is often problem dependent, and also computer architecture dependent. In this talk, we discuss several preconditioning strategies for coupled multi-physics problems including global climate modeling, incompressible flow simulations, fluid-structure interactions, etc. Numerical results will be presented to show the parallel scalability of the approach obtained on supercomputers with thousands or tens of thousands of processor cores.

Authors Index