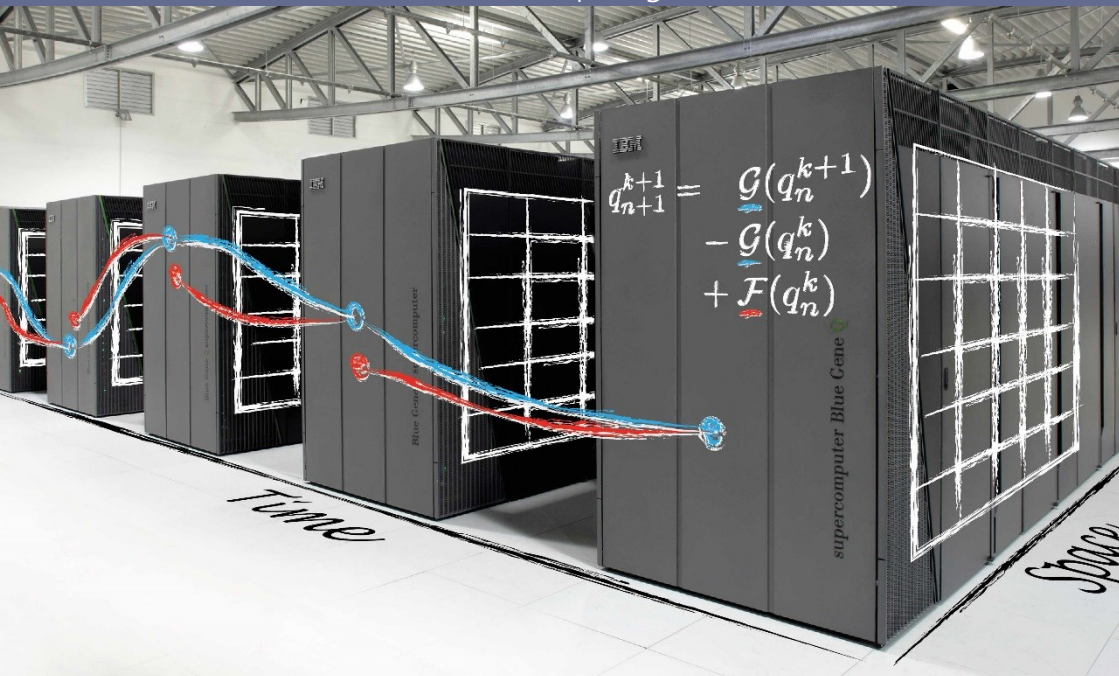




TECHNISCHE
UNIVERSITÄT
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Institute of Scientific Computing



PinT2015

4th Workshop on Parallel-in-Time-
Integration

27-29 May 2015

Technische Universität Dresden

www.tu-dresden.de/pint2015

Organisation

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Schedule

Wednesday, May 27, 2015

09:00 – 13:00	Registration
13:00 – 14:00	Martin Arnold Functional Mockup Interface (FMI): A framework for coarse-grained parallel time integration in nonlinear system dynamics
14:00 – 14:30	Coffee Break
14:30 – 15:00	Andreas Kreienbuehl Time parallel simulation of black hole formation
15:00 – 15:30	Stefan Findeisen Parallel and Adaptive space-time Computation of Maxwell's Equations
15:30 – 16:00	Olga Mula Towards a Fully Scalable Balanced Parareal Method: application to Neutronics
16:00 – 16:30	Coffee Break
16:30 – 17:00	Jacob B. Schroder Multigrid Reduction in Time: A Flexible and Scalable Approach
17:00 – 17:30	Stephanie Friedhoff Multigrid approaches for parallel-in-time integration
17:30 – 18:00	Dieter Moser A multigrid perspective on PFASST
19:00 – 22:00	Informal Meeting at “Watzke am Ring”

Thursday, May 28, 2015

09:00 – 10:00	Hilary Weller Semi-implicit solutions of the fully compressible Euler equations with curl-free pressure gradients
10:00 – 10:30	Coffee Break
10:30 – 11:00	Thomas Slawig A parareal algorithm applied on the computation of periodic states in marine ecosystems
11:00 – 11:30	Teresa Beck In-Time-Parallelization of Atmospheric Chemical Kinetics
11:30 – 12:00	Innocent Niyonzima Time-parallel multiscale finite element method for field computation of eddy current problems
12:00 – 13:30	Lunch Break
13:30 – 14:30	Beth A. Wingate Solving Highly Oscillatory Systems of Equations - locally asymptotic parallel-in-time
14:30 – 15:00	Coffee Break
15:00 – 15:30	Martin Stoll A Low-Rank in Time Approach to PDE-Constrained Optimization
15:30 – 16:00	Dalibor Lukas Parallel Time-Domain Boundary Element Method for 3-Dimensional Wave Equation
16:00 – 16:30	Andreas Naumann Simulation of coupled machine components with ParaExp
18:00 – 21:00	Conference Dinner

Friday, May 29, 2015

09:00 – 10:00

Martin J. Gander
Direct Time Parallel Solvers

10:00 – 10:30

Coffee Break

10:30 – 11:00

Benjamin Ong
Revisionist Integral Deferred Correction with Adaptive
Stepsize Control

11:00 – 11:30

Martin Köhler
Solving Differential Matrix Equations using Parareal

11:30 – 12:00

Nabil R. Nassif
Adaptive Parallel-in-Time Method to Solve second-
order Ordinary Differential Equations

12:00 – 13:30

Lunch Break

13:30 – 14:30

Michael L. Minion
PFASST: Past Present And PFuture

14:30 – 15:00

Coffee Break

15:00 – 16:00

Daniel Ruprecht, Robert Speck
Discussion: Future Direction of the PinT Workshop
Series

16:00 – 16:30

Closing

Impressions



Abstracts

Functional Mockup Interface (FMI): A framework for coarse-grained parallel time integration in nonlinear system dynamics

Martin Arnold, Martin Luther University Halle-Wittenberg

Block structured coupled systems offer a large potential for coarse grain parallelization in time integration. Following a *co-simulation* approach, the data exchange between subsystems is restricted to discrete synchronization points in time. In each macro step, the subsystems are integrated separately by their own integrators using micro time step sizes that may be adapted to the subsystem's time scale. All terms that connect two or more subsystems are substituted by suitable approximations being based on data from previous and current synchronization points.

The *Functional Mockup Interface for Model Exchange and Co-Simulation (FMI)* provides an industrial standard for scheduling such co-simulation algorithms and for the data exchange between slave subsystems and the master algorithm in block structured network models. In FMI, the synchronization points and macro steps are known as communication points and communication steps. FMI supports variable communication step sizes, higher order signal extrapolation for the data exchange between subsystems and the evaluation of Jacobian matrices of all coupling terms.

In the talk, we will give an introduction to FMI and will discuss numerical aspects like zero stability and convergence, variable communication step sizes, communication step size control and linearly implicit stabilization techniques in co-simulation. Some applied problems will illustrate the benefits of the co-simulation approach in the application to coupled systems with different time scales.

Semi-implicit solutions of the fully compressible Euler equations with curl-free pressure gradients

Hilary Weller, University of Reading

Long, stable and accurate time-steps are important for models of the atmosphere to enable efficient weather and climate predictions. This has motivated the use of semi-implicit, semi-Lagrangian models. However semi-Lagrangian techniques appears not to be ideal for the next generation of models for modern computers. Some new numerical methods are presented that enable long, stable time-steps without the non-local communication of semi-Lagrangian. Sub time-stepping is used for advection and acoustic and gravity waves are treated implicitly without the need for mean and perturbation variables.

In addition, a new technique for modelling flow over orography using terrain following layers is introduced which guarantees curl-free gradients implying that the pressure gradient term is not a spurious source of vorticity. This mimetic property leads to better hydrostatic balance and better energy conservation.

Results with large Courant numbers and strong stratification are presented which demonstrates the validity of the sub-cycling of advection and the implicit treatment of gravity waves.

Solving Highly Oscillatory Systems of Equations - locally asymptotic parallel-in-time

Beth A. Wingate, University of Exeter
Terry Haut, Los Alamos National Laboratory
Jared Whitehead, Brigham Young University

In this talk I will present an algorithm for parallel-in-time for highly oscillatory PDEs and show results with the shallow water equations, a model used as a benchmark for weather and climate models. This algorithm is inspired by a mathematically rigorous understanding of the method of multiple time scales by Schochet (1994), Embid and Majda (1998), and others. I will describe the relationship of this theory to the new algorithm and show that the parallel speed-up increases as the time scale separation increases which results in an arbitrarily greater efficiency gain relative to standard numerical integrators. I will also present numerical experiments that demonstrate the parallel speed up is more than 100 relative to exponential integrators such as ETD RK4 and more than 10 relative to the standard parareal method with a linearly exact coarse solver. Finally I will show that the method also works in the absence of time scale separation, allowing for the method to work in different model regimes. In order to begin a discussion about how this method will work on parallel machines I will introduce a new method for computing linear propagators in a very parallel-way and will present some questions about the type of parallelism an algorithm like this could have for heterogeneous computing architectures.

Direct Time Parallel Solvers

Martin J. Gander, Université de Genève

Most methods for the parallel solution in time of evolution problems are iterative in nature. It is however also possible to devise parallel solvers in time which are not iterative. I will explain in my presentation five such methods:

- 1) For small scale parallelization, which is very useful on today's multicore architectures, I will show the early parallel predictor corrector methods of Miranker and Liniger (1967), and the block implicit one step methods of Shampine and Watts (1969), followed by the more recent Revisionist Integral Deferred Correction methods (RIDC) which can give high order accurate solutions on multicore architectures in the same wall clock time as a sequential low order integration method would take.
- 2) Worley (1991) proposed to make multigrid waveform relaxation methods more time parallel by using cyclic reduction for the solution of the scalar time dependent ODEs needed in the smoother. This way one can get close to the information theoretically optimal parallel complexity.
- 3) One can also use a Laplace transform in time and a quadrature rule to approximate the inverse transform, like proposed in Sheen, Sloan and Thomée (1999). The transformed problems at the quadrature nodes can then all be solved in parallel.
- 4) A different idea proposed by Maday and Ronquist (2008) is the diagonalization of the time stepping matrix, provided variable time steps are used. I will show precise error estimates for this method, where round-off error and truncation error need to be balanced for the method to be successful.
- 5) I will finally also explain the ParaExp algorithm for linear problems, which is based on an overlapping decomposition of the time interval with complete overlap and rational Krylov approximations of the matrix exponential. This method is very successful also for linear wave propagation problems.

PFASST: Past Present And PFuture

Michael L. Minion, Lawrence Berkeley National Lab

This talk will give an overview of the Parallel Full Approximation Scheme in Space and Time (PFASST) introduced by Emmett and Minion in 2012. I will discuss the origins of the method and how it relates to other parallel-in-time schemes such as parareal and space-time multigrid methods. Next I will give a summary of recent extensions of the basic algorithm to improve the efficiency and broaden the applicability PFASST. Finally, I will give some opinions on what the future holds for PFASST and parallel-in-time schemes in general.

Time parallel simulation of black hole formation

Andreas Kreienbuehl, USI Lugano

Pietro Benedusi, USI Lugano

Daniel Ruprecht., USI Lugano

Rolf Krause, USI Lugano

An application of the Parareal method to Einstein's equations for spherical, gravitational collapse of a massless scalar field is presented and discussed. We show that Parareal captures the correct black hole formation event and generates the proper mass scaling law. Moreover, if the computational load is properly balanced in time, Parareal features speedup when compared to the serial two-step Lax-Wendroff Richtmyer scheme. As we are using a two-level approach in both space and time, we furthermore analyze the influence of the spatial interpolation. Finally, the efficiency of different Parareal implementations is compared with respect to energy consumption.

Parallel and Adaptive space-time Computation of Maxwell's Equations

Stefan Findeisen, Karlsruhe Institute of Technology
Christian Wieners, Karlsruhe Institute of Technology
Willy Dörfler, Karlsruhe Institute of Technology

We consider the parallel simulation of electromagnetic waves described by linear Maxwell's equations. We use a tensor product ansatz with a discontinuous Galerkin finite element method for the spatial discretization and a Petrov-Galerkin discretization in time. The upwind flux is used to approximate continuity across cell faces. Hence we get a continuous ansatz space and discontinuous test space in time, whereas ansatz and test space are both discontinuous in space.

The computational domain is decomposed into space-time cells and distributed among different processes, to solve the complete problem in parallel.

Our method is p-adaptive with different polynomial degrees in space and time in every space-time cell. A dual weighted goal-oriented error estimator is realized for the adaptive selection of the polynomial degrees on every space-time cell. Hence we are able to reduce the error towards a given error functional (e.g. energy error functional) in a space-time region of interest during several adaptive iterations.

Since the discretization is implicit in time, no CFL limitation applies. The linear advection equation is used as a test case for a transport problem to show the reliability of the method and the error estimator. First results in 2+1 dimensions for Maxwell's equations with more than 100 million space-time degrees of freedom on 1000 processors illustrate the parallel efficiency of the method.

Towards a Fully Scalable Balanced Parareal Method: application to Neutronics

*Yvon Maday, Université Pierre et Marie Curie & Brown University &
Institut Universitaire de France*

Olga Mula, RWTH-Aachen University

Mohammed Kamel Riahi, New Jersey Institute of Technology

In the search for new parallel directions for the efficient exploitation of large scale systems, the parallelization of the time domain is a very promising approach since it could dramatically reduce computing times in the resolution of time-dependent PDE's when other parallelization methods (like, e.g., spatial domain decomposition) reach saturation. However, all the existing methods for parallelizing the time variable present in practice severe efficiency limitations that “spoil” the huge potential of the idea. This article is a contribution towards overcoming this major obstruction by exploiting the idea that the numerical schemes to parallelize time could be coupled to other schemes that are needed to solve the PDE. Our main focus will be on improving the performances of the parareal in time algorithm in the case where the propagation of the so-called fine solver requires iterative fixed-point schemes at each time step. We present a parareal scheme in which these internal iterations are truncated (i.e. not converged) at each time step but in which convergence is still achieved across the parareal iterations. After a convergence analysis, we present some numerical results dealing with the application of the scheme to accelerate the time-dependent neutron diffusion equation in a reactor core. The numerical results show a significant improvement of the performances with respect to the plain parareal algorithm, which is an important step towards making the parallelization of time be a fully competitive option for the exploitation of massively parallel computers.

Multigrid Reduction in Time: A Flexible and Scalable Approach

Jacob B. Schroder, Lawrence Livermore National Lab

Robert Falgout, Lawrence Livermore National Lab

Tzanio Kolev, Lawrence Livermore National Lab

Ulrike Yang, Lawrence Livermore National Lab

Veselin Dobrev, Lawrence Livermore National Lab

Anders Petersson, Lawrence Livermore National Lab

Benjamin O'Neill, University of Colorado

Stephanie Friedhoff, KU Leuven

Scott MacLachlan, Memorial University

In this talk, we examine an optimal-scaling parallel time integration method, multigrid-reduction-in-time (MGRIT). MGRIT applies multigrid to the time dimension by solving the (non)linear systems that arise when solving for multiple time steps simultaneously. The result is a versatile approach that is non-intrusive and wraps existing time evolution codes. MGRIT allows for various time discretizations (e.g., Runge-Kutta and multistep) and for adaptive refinement/coarsening in time and space. Non-linear problems are handled through full approximation scheme (FAS) multigrid. Our software implementation in the XBraid library (llnl.gov/casc/xbraid) and practical results for a variety of problems will be presented, e.g., explicit/implicit time integration, non-linear diffusion and compressible Navier-Stokes.

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Multigrid approaches for parallel-in-time integration

Stephanie Friedhoff, KU Leuven

Multigrid and related multilevel methods are the approaches of choice for solving the linear systems that result from the discretization of a wide class of PDEs. One feasible approach for doing effective parallel-in-time integration is also through some kind of multilevel method. There are two approaches for extending classical multigrid methods to include the time dimension: multigrid only in time and space-time multigrid. The multigrid-reduction-in-time (MGRIT) algorithm [Falgout et. al., SIAM J. Sci. Comput., 36 (2014), pp. C635-C661] employs a non-intrusive semicoarsening strategy using coarsening only in the time dimension. In space-time multigrid (STMG) [Horton and Vandewalle, A space-time multigrid method for parabolic PDEs, SIAM J. Sci. Comput., 16 (1995), pp. 848-864], time is treated as simply another dimension in the grid. The method is characterized by an adaptive parameter-dependent coarsening strategy, employing either semicoarsening in space or in time on the different grid levels in the multigrid hierarchy.

In this talk, we compare the different approaches for integrating multigrid concepts into time-evolution algorithms.

A multigrid perspective on PFASST

Dieter Moser, Jülich Supercomputing Centre

The Parallel Full Approximation Scheme in Space and Time (PFASST) is a time-parallel iterative method, which already shows promising results for many use cases. However, a solid and reliable mathematical foundation is still missing. In this talk, we explore the strong connection between PFASST and classical multigrid schemes. We show that, under certain assumptions, the PFASST algorithm for linear problems can be conveniently and rigorously described as a multigrid-in-time. Since multigrid methods were studied extensively in the past, a lot can be gained from this connection for a better understanding of PFASST. We focus on the application of Local Fourier Mode Analysis and show first results for several examples.

A parareal algorithm applied on the computation of periodic states in marine ecosystems

Thomas Slawig, Christian-Albrechts-Universität zu Kiel
Jaroslav Piwonski, Christian-Albrechts-Universität zu Kiel
Björn Peiler, Christian-Albrechts-Universität zu Kiel

We used a parareal algorithm for the computation of steady periodic annual cycles of a 3-D marine ecosystem (or biogeochemical) model coupled to pre-computed ocean transport. Overall goal of this kind of simulation is to perform a model calibration or parameter identification. This is usually done by an optimization algorithm, which itself requires a high number of simulation runs. The usual computation of one steady periodic solutions takes up to 10'000 years model time, each of which requires about 3'000 time-steps. The simulation model is a discretized system of transport equations coupled by non-linear and non-local reaction terms. For 3-D simulations, the model is already spatially parallelized by domain decomposition and MPI. To achieve additional performance gain, a parareal algorithm based on a coarser time-stepping was applied. We show first results of this strategy for the mentioned application, and discuss further options for exploiting parallelization in time.

In-Time-Parallelization of Atmospheric Chemical Kinetics

Teresa Beck, Universität Heidelberg

The simulation of atmospheric chemical kinetics is a time-consuming part within typical air quality models. The chemical kinetics are described by systems of stiff ordinary differential equations, which are characterized by the presence of a wide range of time-scales. This poses severe stability restrictions to a time-stepping scheme. Typically, implicit adaptive time-stepping schemes are used for their numerical solution. Since such schemes inhere only a limited potential of parallelism within the calculation of each time-step, a parallelization across time is promising. To speed-up the numerical simulation, we choose the parareal algorithm. Its application to atmospheric chemical kinetics is challenged by the presence of stiffness. We present a combined application of model reduction and the parareal algorithm to stiff problems arising from atmospheric chemical kinetics.

Time-parallel multiscale finite element method for field computation of eddy current problems

Innocent Niyonzima, Technische Universität Darmstadt

Time-domain parallel methods are becoming increasingly important for engineering applications. The use of these methods allow to speed-up numerical computations thanks to the parallel architecture of modern computers. The modeling of eddy currents problems in electromagnetism leads to the resolution of (stiff) parabolic/elliptic partial differential equations often involving composite materials for which the numerical solution can be naturally obtained by the Parareal method. In this contribution we propose the implementation of a Parareal method for solving the differential algebraic equations resulting from space discretization of the weak formulations of eddy currents problems involving composite materials. The method combines ideas from the heterogeneous multiscale method (HMM) and the Parareal method. A coarse macroscale problem defined on coarse spatial is solved using a coarse temporal grids and many finescale mesoscale problems are defined on fine meshes around Gauss points and solved using a fine temporal grids. Details of implementation (the coupling between the macroscale and the mesoscale problems) will be provided in the full contribution.

A Low-Rank in Time Approach to PDE-Constrained Optimization

*Martin Stoll, Max Planck Institute for Dynamics of Complex Technical
Systems Magdeburg
Tobias Breiten, University of Graz*

The solution of time-dependent PDE-constrained optimization problems is a challenging task in numerical analysis and applied mathematics. Space-time all-at-once discretizations and corresponding solvers provide efficient methods to robustly solve the arising discretized equations. One of the drawbacks of this approach is the high storage demand for the vectors representing the discrete space-time cylinder. Here we introduce a low-rank in time technique that exploits the low-rank nature of the solution and hence enables a drastic storage reduction regarding the space-time problem. The theoretical foundations for this approach originate in the numerical treatment of matrix equations and can partly be carried over to PDE-constrained optimization. We illustrate how different problems can be rewritten and used within a low-rank Krylov subspace solver with appropriate preconditioning.

Parallel Time-Domain Boundary Element Method for 3-Dimensional Wave Equation

Dalibor Lukas, Technical University of Ostrava

Alexander Veit, University of Chicago

Michal Merta, Technical University of Ostrava

Jan Zapletal, Technical University of Ostrava

We present a boundary element method for 3-dimensional sound-hard scattering. It relies on an indirect formulation for the retarded double-layer potential introduced by Ha Duong and on smooth time ansatz functions recently proposed by Sauter and Veit. The latter allows for an efficient use of Gauss quadrature within the assembly of the resulting boundary element system matrix. The assembling process is implemented in parallel and we numerically document its scalability. Further, a heuristical preconditioner, which accelerates flexible GMRES iterations, is presented. The efficiency of our approach is documented for a problem on a sphere with known analytical solution as well as for a scattering from a real-world geometry.

Simulation of coupled machine components with ParaExp

Andreas Naumann, TU Dresden
Michael Klöppel, TU Dresden
Jörg Wensch, TU Dresden

The accuracy requirements in recent mass production processes demand new compensation techniques and structures of tool machines. To achieve these requirements, one has to know the thermo-elastic behavior and interaction of the coupled components during the design phase. We apply an extension of the ParaExp-method on the linear time varying ODE for semidiscretized coupled heat equations.

Revisionist Integral Deferred Correction with Adaptive Stepsize Control

Benjamin Ong, Michigan Tech University

Adaptive step-size control is a critical feature for the robust and efficient numerical solution of IVPs. We discuss various strategies and implementation issues that arises when incorporating adaptive step-size control into revisionist integral deferred correction methods, a family of parallel-in-time integrators.

Solving Differential Matrix Equations using Parareal

Martin Köhler, Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg

Norman Lang, Technische Universität Chemnitz

Jens Saak, Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg

Differential matrix equations such as the Differential Riccati Equation (DRE)

$$E^T \dot{X} E = A^T X E + E^T X A + C^T C + E^T X B B^T X E$$

or the Differential Lyapunov Equation (DLE)

$$E^T \dot{X} E = A^T X E + E^T X A + C^T C$$

are tools in the fields of optimal control and model order reduction of dynamical systems. Here $A, E \in R^{n \times n}$ are the square system matrices, while the output matrix $C \in R^{m \times n}$ and input matrix $B \in R^{n \times p}$ are allowed to be rectangular. Thus, the solution $X \in R^{n \times n}$ is also square and usually densely populated.

The origin of the system matrices (A, E) leads to stiff problems. Therefore, here we solve both types of equations with Rosenbrock-type integrators. These implicit methods require the solution of one algebraic Lyapunov equation per Rosenbrock stage in each time step. Since the order of the method roughly speaking coincides with the number of stages, using higher order methods, this results in high computational costs. Furthermore, the most expensive operations, to solve the algebraic Lyapunov equations, do not scale across many CPU cores and in large parts run strictly sequential (roughly $60n^3$ out of $63n^3$ flops).

In order to accelerate the solution process on a fine time grid we surround the Rosenbrock-methods by a standard pipelined parareal

approach for shared and distributed memory systems. In our contribution we show the runtime results of current implementations and describe open problems, we recognized during the development.

Adaptive Parallel-in-Time Method to Solve second-order Ordinary Differential Equations

*Nabil Rafic Nassif, American University of Beirut
Noha Makhoul Karam, Université Saint Joseph, Beirut*

In recent works, ([13] and [14]), we have used an adaptive parallel-time (APTI) approach for solving the initial value problem:

$$\frac{dY}{dt} = F(t, Y), \quad t > 0, \quad Y(0) = Y_0, \quad Y_0, Y(t) \in R^n,$$

implementing such method to solve a number of applications. The APTI method generates automatically non-regular time grids $\{ [T_{n-1}, T_n] \mid n = 1, \dots, N \}$ and predict, in parallel, initial data $Y_{a,n-1}$ that approximates $Y(T_{n-1})$ at the beginning, T_{n-1} , of each slice of the coarse grid. Parallel time integration follows then through the partition of the ODE problem into a sequence of ODE shooting value problems, each defined on a time slice of the coarse grid:

$$\frac{dY}{dt} = F(t, Y), \quad t \in (T_{n-1}, T_n], \quad Y(T_{n-1}) = Y_{a,n-1}$$

This approach is consistent with those used since the 90's, starting with [2] and [4], followed by the very popular parareal algorithm which is found in a large number of papers such as [5], [7], [6], and [10].

In this paper, we illustrate the method on 2-nd order ODE's, such as the membrane problem:

$$\begin{cases} y'' - b|y'|^{q-1} y' + |y|^{m-1} y = 0, & t > 0, \\ y(0) = y_{1,0}, & y'(0) = y_{2,0}, \end{cases}$$

which has singular and oscillatory behavior on $(0, \infty)$.

We show that an appropriate end-of-slice condition at T_n is given by:

$$y'(T_n) = |y(T_n)|^{\frac{2}{m+1}}.$$

Followed by the change of variables:

$$t = T_{n-1} + \beta_n s, \quad y(t) = Y(T_{n-1})(I + Z(s)),$$
$$\beta_n = |y(T_{n-1})|^{\frac{1-m}{2}},$$

we obtain “similarity properties” between the local systems defined on the time slices $\{[T_{n-1}, T_n] \mid n = 1, 2, \dots, N\}$ (as in [8], [9] and [11]). This allows to devise and implement the APTI parallel algorithm that results in high speed-ups, tested on a 2, 4 and 8 cores machine.

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