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2015

UNIVERSITÀ DEL SALENTO

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Scientific Program - Timetable

Sunday 22	Time	Monday 23	Tuesday 24	Wednesday 25	Thursday 26	Friday 27
	9:15		Contributed sessions (15 in parallel)	Plenary Lecture Moritz Diehl	Contributed sessions (15 in parallel)	Contributed sessions (14 in parallel)
	9:30					
	9:45					
	10:15	Registration		von Mises prize lecture		
	10:30					
	10:45					
	11:15		Coffee Break	Coffee Break	Coffee Break	Coffee Break
	11:30					
	11:45					
	12:15		Plenary Lecture Thomas Böhlke	General Assembly	Plenary Lecture Ferdinando Auricchio	Contributed sessions (11 in parallel)
	12:30					
	12:45					
	13:15	Opening	Lunch	Lunch	Lunch	
	13:30					
	13:45	Univ. Chorus Performance				Closing
	14:15	Prandtl Lecture Keith Moffatt	Plenary Lecture Enrique Zuazua	Contributed sessions (15 in parallel)	Plenary Lecture Daniel Kressner	
	14:30					
	14:45					
	15:15	Plenary Lecture Giovanni Galdi	Plenary Lecture Nikolaus Adams		Plenary Lecture Stanislaw Stupkiewicz	
	15:30					
	15:45					
Registration pre-opening	16:15	Coffee Break	Coffee Break Poster session	Coffee Break	Coffee Break Poster session	
	16:30	Minisymposia & Young Reseachers' Minisymposia (10 in parallel)	Contributed sessions (14 in parallel)	Contributed sessions (15 in parallel)	Contributed sessions (15 in parallel)	
	16:45					
	17:15					
	17:30					
	17:45					
	18:15		Public lecture Francesco D'Andria			
	18:30					
	18:45					
	19:15	Opening reception at Castle of Charles V				
	19:30					
	19:45					
	20:15			Conference dinner at Hotel Tiziano		
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GAMM 2015

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S22: Scientific computing

Scientific Computing is concerned with the efficient numerical solution of mathematical models from both science and engineering. The field covers a wide range of topics: from mathematical modeling over the development, analysis and efficient implementation of numerical methods and algorithms to software and finally application for the solution of complex real-world problems on modern computing systems. This interdisciplinary field combines approaches from applied mathematics, computer science and a wide range of applications in which in-silico experiments play an increasingly important role.

Micro-macro parareal methods for multiscale problems

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We introduce a micro-macro parareal algorithm for the time-parallel integration of multiscale-in-time systems. The algorithm first computes a cheap, but inaccurate, solution using a coarse propagator (simulating an approximate slow macroscopic model), which is iteratively corrected using a fine-scale propagator (accurately simulating the full microscopic dynamics). This correction is done in parallel over many subintervals, thereby reducing the wall-clock time needed to obtain the solution, compared to the integration of the full microscopic model over the complete time interval. We provide a numerical analysis of the algorithm for a prototypical example of a micro-macro model [1], namely singularly perturbed ordinary differential equations, and illustrate the method for problems arising in climate modeling and molecular dynamics.

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Adaptive space time finite element methods for dynamic nonlinear thermomechanical coupled problems

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In this contribution, we consider nonlinear thermomechanical coupled problems of the following type: Find a displacement field u and a temperature distribution θ, which fulfill the equation of motion with a temperature dependent stress field and the heat equation including a heat source depending on the displacement:

$$\begin{aligned} \rho\ddot{u} - \operatorname{div}(\sigma(u,\theta)) &= f \\ \rho c_p \dot{\theta} - \operatorname{div}(\kappa(\theta)\nabla\theta) &= g(u) \end{aligned}$$

Additionally, appropriate intial and boundary conditions have to be specified. The continuous model is discretized with a space time Petrov Galerkin method using continuous and piecewise d-linear basis functions in space and time, which can be reduced to a time stepping scheme due to the discontinuous piecewise constant temporal test functions, see for instance [1]. The resulting coupled system in each time step is solved by a staggered scheme. The aim is to control the discretization error as well as the error in the solution scheme in a nonlinear goal functional. To this end, we use the dual weighted residual (DWR) method. In detail, we combine the ideas from [1] for goal oriented error estimation in nonlinear time dependent problems and from [2] for balancing discretization and numerical error in static problems. The discretization error is measured by the usual DWR techniques discussed for time dependent problems, e.g., in [1], while the numerical error is estimated by testing the residuum with the discrete dual solution, cf. [2]. However, the error estimator can only be evaluated after solving the complete primal and dual problem. Thus, we have to design a special solution algorithm. The main idea is to solve the primal problem doing only one step of the staggered solution scheme in each time step. Then the discretization and the numerical error is estimated. If the numerical error is dominant, an additional loop over all time steps including one step of the staggered scheme is executed. Otherwise, the mesh is adaptively refined. By this approach, we can reduce the numerical effort for the accurate solving of thermomechanical problems by adopting the solution scheme to the special needs of the underlying problem and the chosen goal functional.

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Parallel simulation of large scale multibody systems

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Virtual prototyping plays an ever increasing role in the engineering disciplines. Nowadays, engineers can rely on powerful tools like object oriented modeling languages, e.g., Modelica. Models written in this language can be simulated by open source software as well as commercial tools. The advantage of this approach is that the engineers can concentrate themselves on modeling, whereas the numerical intricacies of the simulation are handled by the software. On the other hand the simulations are usually slower than implementations which are parallelized and optimized by hand. This can lead to computation times which are infeasible in practice, e.g., when a real time simulation is necessary for a hardware-in-the-loop simulation.

In this contribution we are concerned with speeding up such automated simulations by parallelization (on desktop hardware as well as HPC systems). We examine the three classical approaches, i.e., parallelism across the system, parallelism across the method and parallelism across the steps. Additionally, the influence of the problem formulation on the simulation time is discussed. We demonstrate what kind of information can be gained from the automatically generated equations and how this information can be used to efficiently speed up the computation. The implemented methods are demonstrated on engineering examples. Furthermore, successful method will be made available in the open source simulation software OpenModelica.

Simulation of coupled machine components on long time scales

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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 discretize the machine components using finite elements. The heat exchange of the components couples the temperature fields, which leads to additional constraints on parallel FEM. The discretization in space leads to a system of coupled ODEs, which are of stiff parabolic type with fast time-varying source terms. We concentrate on numerical methods to solve those equations on large timescales and reduce the timestep restriction to the fast coupling. This includes averaging techniques, as well as parallel in time methods.

Boris–SDC: A high-order Boris integrator

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This talk will introduce and investigate the high-order Boris-SDC method [1] for integrating the equation of motion for electrically charged particles in an electric and magnetic field.

The well-known and widely used Boris scheme [2, 3] is a second-order accurate Lorentz force integrator. Based on the standard velocity-Verlet scheme for molecular dynamics simulations, this approach resolves the seemingly implicit velocity dependence in the equations of motion by exploiting the rotational character of the magnetic field contribution. In doing so, it provides a fully explicit, cheap particle pusher and has become the de-facto standard integration method for this kind of problems. Today, the Boris method is applied in essentially all particle-based plasma physics simulations involving magnetic fields, e.g. in laser-plasma physics algorithms as well as space weather and fusion-related simulations [4].

We extend the second-order method to arbitrary orders of accuracy by coupling the Boris approach with spectral deferred corrections (SDC, [5]). SDC can be considered as preconditioned Picard iteration for computing the solution of a collocation method. In this interpretation, inverting the preconditioner corresponds to a sweep with a low-order method. While common implementations make use of implicit or explicit Euler integrators, we employ velocity-Verlet as base sweeper [6] and incorporate the Boris method as solver for the implicit velocity dependency.

Boris-SDC provides a generic way to extend the classical Boris integrator to a high-order method. Stability, convergence order and conservation properties of the method are demonstrated for different simulation setups. The method reproduces the expected high order of convergence for a single particle and for the center-of-mass of a particle cloud in a Penning trap and shows good long-term energy stability. Besides its high formal order, its attractive properties and ease-of-implementation provide the foundation of a considerably improved approach to particle trajectory integration in electric and magnetic fields. Furthermore, the formal methodology presented here can be understood as a blueprint for the adaptation of other specialized integration methods to SDC.

This method also pioneers upcoming time-parallel integration for this problem. Using SDC-based integrators like the one presented here, the 'parallel full approximation scheme in space and time' (PFASST, [7]) allows to integrate multiple time-steps simultaneously using sweeps of SDC on different levels of a space-time hierarchy. The presented results constitute an important step towards a parallel-in-time Boris integrator.

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Efficient Nested Chebyshev Smoothing

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Chebyshev semi-iteration, as a polynomial smoother, has been shown to be an effective component of a multigrid process, particularly in parallel settings where an estimate of the largest eigenvalue can be obtained efficiently [2]. As a preconditioner, the approach has been shown to be superior even to nested Kyrlov methods as a preconditioner in some cases (namely those when good spectral estimates are available a priori), and can be more effectively analyzed due to its linearity, for fixed spectral estimates [4]. Related to this property is a corresponding benefit in the context of contemporary hybrid HPC architectures: local Chebyshev smoothing can be applied with a single kernel launch on an accelerator device, and computed using recently-developed blocking techniques which increase cache reuse and utilize more of the available arithmetic intensity on modern accelerators; further, these can be used to reduce global communication with a multigrid cycle by performing more aggressive coarsening [1].

We investigate efficiency gains using local Chebyshev smoothing in the context of preconditioning challenging Stokes problems from mantle convection, on a large system with hybrid CPU/GPU nodes. Our recent comparative studies [3] within the PASC GeoPC Project[1] have demonstrated that in practical simulations, "heavy smoothing" can be employed to reduce the amount of communication required, mitigating a bottleneck at extreme scale. We investigate the effects of varying the accuracy of automatic eigenvalue estimates, and examine the effects of combining Chebyshev smoothers hierarchically, as global smoothers, preconditioned by local smoothers working on GPUs.

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Rayleigh Quotient Inverse Iteration with Adaptive Algebraic Multigrid for Lattice QCD

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In lattice Quantum Chromodynamics (lattice QCD) computations, the calculation of physical observables oftentimes requires approximations to the full inverse of very large sparse matrices, i.e., inverses of the lattice Wilson Dirac operator D. Numerical methods used in the Physics community highly demand singular vectors corresponding to smallest singular values of D. In this talk we present a Rayleigh quotient inverse iteration approach in combination with an adaptive algebraic multigrid solver. We show numerical results for medium scale parallelizations of up to 4,192 cores and problem sizes of up to 200,000,000 unknowns.

An Auxiliary Space Type Preconditioner for Simulations in Lattice QCD

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In this talk we motivate, analyze and experimentally validate a new preconditioner for the overlap operator of lattice QCD. Lattice QCD simulations are among today's most demanding supercomputer applications, and substantial resources are spent in these computations. Most frequently, these simulations are based on repeatedly solving systems with the Wilson-Dirac operator $D_W(\kappa)$, a nearest-neighbor discretization of the respective Dirac equation.

From a theoretical point of view, the *overlap operator*

$$D_{ovl} = \rho I + \Gamma_5 \mathrm{sign}(\Gamma_5 D_W(\kappa_{ovl}))$$

is particularly attractive since it respects an important physical property, chiral symmetry, which is violated by other lattice discretizations. From a practical point of view, the overlap operator has the disadvantage that its computational cost can be two orders of magnitude larger than when using standard discretizations due to the occurence of the matrix sign function.

The basic idea of the preconditioner we propose is to use the Wilson-Dirac $D_W(\kappa_W)$ operator to form a preconditioner for the overlap operator. This may be regarded as a variant of the fictitious (or auxiliary) space preconditioning technique that has been used for developing and analyzing multilevel preconditioners for various nonconforming finite element approximations of PDEs. One works with a mapping from the original space to a fictitious space, yielding an equivalent problem that is easier to solve. Preconditioning is then done by (approximately) solving this equivalent problem. The convergence properties of auxiliary space preconditioning depend on the choice of the fictitious space, and its computational efficiency depends, in addition, on the efficiency of the solver used in that space.

For the overlap operator in lattice QCD, choosing its kernel—the Wilson-Dirac operator—as the auxiliary space preconditioner is facilitated by the fact that both operators are defined on the same Hilbert space. In this way, the preconditioner for the former can be constructed using an adaptive algebraic multigrid solver for the latter on the same finite dimensional lattice.

A crucial issue is to establish an optimal connection between the parameters ρ, κ_{ovl} and κ_W. We do so in a theoretical analysis for the case that D_W is normal. Although this is not exactly the case in realistic settings, we show that current smearing techniques indeed drive the Wilson-Dirac operator towards normality, thus providing a motivation why our preconditioner works well in computational practice. We demonstrate that our technique is able to reduce the computational cost for solving systems with the overlap operator substantially, reaching speed-ups of a factor of 10 or more in realistic settings, involving large lattices and state-of-the-art implementations on parallel computers, particularly the JUROPA cluster system at FZ Jülich.

A GPU implementation of the Factored Sparse Approximate Inverse preconditioner for the iterative solution of SPD linear systems

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It is well known that GPUs exhibit significantly higher peak performance than conventional CPUs. However, due to their programming model and microarchitecture, only highly parallel algorithms can exploit their full potential. In this context, the development of effective algorithms for the solution of large and sparse linear systems of equations

$$A\mathbf{x} = \mathbf{b},$$

where A is the system matrix, $\mathbf{x}$ is the solution vector and $\mathbf{b}$ is right-hand-side, is still an open problem. Conjugate gradient-like algorithms are good candidates for this task as they require only sparse matrix-by-vector products, dot products and vector updates, which have all already been implemented successfully on GPUs [4, 5]. However, the performance of any iterative solver is strictly related to the availability of an effective preconditioner, that is, an approximation of A^{-1} which has to be relatively cheap to compute and apply to a vector. The development of effective preconditioners on GPUs is not straightforward and several attempts have already been made (see, e.g., [1, 3]). In the present contribution, we propose the Factored Sparse Approximate Inverse (FSAI) [2], which, with its inherent parallelism, is an optimal preconditioner for the conjugate gradient solver. FSAI gives an explicit approximation of A^{-1} in factored form, i.e. $GG^T \simeq A^{-1}$, and is computed by minimizing the matrix function

$$\|I - GL\| \rightarrow \min \tag{1}$$

over all the matrices G having a prescribed lower triangular sparsity pattern. In (1) L is the exact lower triangular factor of A, which is not required to be explicitly known during the computation of G. While the FSAI application to a vector involves only sparse matrix-by-vector products, a GPU-based implementation requires a nontrivial recasting of multiple computational steps. One of the main issues is to find a suitable data mapping between threads and data in order to exploit the massive GPU parallelism. To that purpose, we resorted to a solution that we successfully exploited in a pretty different context [6]. The other issue is the need of carrying out the Cholesky decomposition on large batches of small systems. We experimented with different strategies and obtained the best performances by using a block of threads per system and performing the factorization exclusively in register memory. We illustrate our experience with the full porting of a parallel FSAI preconditioner on NVIDIA GPUs; experiments show a significant speedup over the CPU-only, OpenMP-based implementation.

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Finite Volume Methods for Sound-Advection-Buoyancy Systems

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The simulation of atmospheric dynamics relies on the numerical solution of the Euler equations. We consider here buoyancy-sound-advection systems for stratified fluids. These systems exhibit wave type solutions which impose CFL-based restrictions on the time step size. Buoyancy, sound and advection cause seperate restrictions, each on their own scale. We develop Finite Volume Methods where a splitting approach allows different treatment of fast and slow waves. The methods are optimized with respect to order and maximum stable CFL numbers. Different scenarios for the scales of sound, advection and buoyancy are discussed.

HPC methods for structured inverse modeling in diffusive processes

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In many applications, which are modeled by diffusion processes, there is a small number of different materials involved with distinct boundaries. It is thus reasonable not only to estimate the permeability parameter itself but also the contour of the spatial distribution by methods of shape optimization. Depending on the complexity of the interfaces, this requires the solution of several very large systems of equations resulting from fine discretizations of PDE systems.

It is thus obligatory to develop efficient software for supercomputers that guarantees scalability also for problems where most degrees of freedom are located on interfaces. Here it turns out that the efficiency of the optimization algorithm strongly depends on the applied load balancing technique since there are many costly operations which are only computed on the surfaces to be optimized. It is thus discussed how load balancing can be adapted such that surfaces in the FEM mesh are also evenly distributed among processors.

This talk introduces a limited memory BFGS approach for shape optimization in diffusive flow processes. It is shown that superlinear convergence can be achieved which is a significant speedup against optimizations based only on shape gradients. These techniques are utilized in order to fit a model of the human skin to data measurements and not only estimate the permeability coefficients but also the shape of the cells.

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Using Automatic Differentiation to Create Sparse Jacobians for the Solution of Nonlinear Partial Differential Equations

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During the development of numerical simulation software, a number of situations arise, where it becomes necessary to differentiate either mathematical terms or the output of a program function. One very important example is the solution of nonlinear partial differential equations (PDE). During the linearization step needed to solve the discretized form of the equations, e.g., based on the Newton-Raphson algorithm, the Jacobian of the residual with respect to the unknown field variables is needed:

$$\frac{\partial \mathbf{F}(\mathbf{u}_k)}{\partial \mathbf{u}} \cdot \Delta \mathbf{u}_{k+1} \;=\; -\mathbf{F}(\mathbf{u}_k).$$

Although the manual calculation of the Jacobian (or a close approximation thereof) is a viable choice, the resulting code will always be specific to a single PDE and discretization scheme, which may render it difficult to adapt the implementation to a new simulation model. In addition, the program code to calculate the derivative will often be difficult to read, a circumstance, which can invite errors in the implementation. A simple method of validating the analytical derivation as well as the implementation is often lacking. While, e.g., the successful minimization of the residual can be taken as an indication that the derivative is correct, it does not conclusively prove it.

In recent years, a lot of research has been carried out in the field of automatic differentiation (AD). Such methods allow the mathematical differentiation of program functions, which may or may not have a closed analytical representation. In order to take a first step towards utilizing AD in our in-house finite element software XNS, which is written in Fortran, we automatized the creation of the Jacobian for a Newton-Raphson iteration with the software Tapenade [1]. As a result, the task of implementing a new set of equations is reduced to the effort of calculating the residual of the discretized weak form.

As a test case we used the viscoelastic fluid equations [2], which were chosen due to their significant nonlinearities. The equations are discretized in XNS using the GLS-stabilized finite element method. We will discuss the various problems that we had to solve on our path towards a useful result. Most importantly, we will present the different approaches that we explored as a means of exploiting the sparsity of the Jacobian matrix in an efficient manner. We will conclude by showing that we were able to create a method, which is already reliable and flexible, and opens up possibilities to either quickly and easily implement new equations or to validate an existing manual implementation of the derivative.

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Multiple-output variable fidelity modeling of vehicle aerodynamics under geometric shape variations

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Variable-fidelity modeling (VFM), sometimes also termed multi-fidelity modeling, refers to the exploitation of two or more data layers of variable accuracy in order to construct an inexpensive emulator of a given high-order numerical model. In practical applications, this situation arises, when simulators of different accuracy for the same physical process are given and it is assumed that many low-fidelity sample points are affordable, but the high-fidelity model is extremely costly to assess.

More precisely, the VFM objective is to construct a predictor function based on the variable-fidelity sample data sets, which *interpolates* the primary sample data driven by the trend indicated by the secondary data, where it is tried to use as few high-fidelity sample points as possible to achieve a desired level of accurancy.

While previous work on VFM has focused on scalar-valued multiple-input-single-output models [1, 2], in this work, we extend the approach to large-scale nonlinear multiple-input-*multiple-output* models. To this end, we combine the VFM with the method of proper orthogonal decomposition. In particular, we are interested in the approximation of complete field solutions of dimensions ranging from several hundreds of thousands up to several millions as they arise from the spatial discretization of partial differential equations in industrial applications.

The method is illustrated on an automotive computational fluid dynamics problem, where the objective is to predict the complete flow-field corresponding to a given spatial discretization under multi-parameter variations of the shape of the rear of the car. Fully and partly converged flow solutions act as data layers of high- and low fidelity, respectively. The approach is non-intrusive in the sense that the underlying flow solver acts as a black box function and no intrinsic modifications are required.

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Sensitivities calculations for unsteady flow problems

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In this work we present an efficient approach for the calculation of the sensitivities in the case of unsteady problems like the compressible transient high-speed flows around a wing-section. The sensitivities are of the lift and pitching moment dimensionless coefficients and are determined with respect to the time-dependent boundary conditions. These sensitivities are necessary for the solution of inverse problems or for the synthesis of an active control law. If the number of design parameters is large, the adjoint method is typically used because the cost of computing the sensitivities does not depend on the number of design parameters. However, the underlying partial differential equations of the optimization problems are usually for a steady state, even their solution is obtained using a time-dependent numerical algorithm. The so-called one-shot approach introduced by Ta?asan (1991) the optimization problem is solved simultaneously with the governing equations. An iterative process called piggy-back allows the calculation of the state and adjoint variable at each iteration, followed by the upgrade of the design parameters. The extension of the one-shot method to unsteady problems is of crucial importance, due to the efficiency of the computational process. This has been conceptually done by Gauger and all (2013). In this work, we first derive the adjoint equations for the Euler model. The emphasis is on the correct formulation of the adjoint boundary conditions, in the framework of the imposition of the unsteady boundary conditions. Finally, we propose an algorithm for the efficient solution of the forward and adjoint problem simultaneously, by using a piggy-back iteration process inside an one-shot method to advance in time.

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EWE – A coupled electro-mechanical heart model in the general purpose FEM framework MOOSE

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The talk will present ongoing efforts on the development of a coupled electro-mechanical heart model called EWE, which are part of the Center for Computational Medicine in Cardiology in Lugano. The model is implemented using the open source general purpose C++ finite element framework MOOSE [1], which is based on the libMesh library [2] and has been used for a number of different applications in a broad range of sicentific fields [3].

So far, EWE comprises a nonlinear mechanical model coupled with a monodomain electrocardiac model. Cellular ion channels are represented through the model by Bernus et al. [4]. Using the MOOSE framework resulted in a major acceleration of software development: Although only a few months old, coupled simulations of electrocardiology and cardiomechanics are now possible with EWE and the talk will show some preliminary results. For parallelization, the code relies on the widely used and well developed solver library PETSc [5]: Scaling benchmarks on a Linux cluster and a state-of-the-art Cray supercomputer will be presented and discussed and the further directions of development for EWE will be outlined.

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Enriching Finite Elements with meshless nodes in structural mechanics

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The automatic generation of meshes for the Finite Element method can be an expensive computational burden, especially in structural problems with localized stress peaks. The use of meshless methods can address such an issue, as these techniques do not require the existence of an underlying connection among the nodes selected in a general domain. However, a thoroughly meshfree technique can be computationally quite expensive. Usually, the most expensive tasks rely in identifying the nodal contacts and computing the Galerkin integrals.

In this communication we advance a novel hybrid technique that blends Finite Elements with the Meshless Local Petrov-Galerkin method (MLPG, [1]) with the aim at exploiting the most attractive properties of each procedure. The idea is based on the original proposal by Ferronato et al. [2] and relies on the use of the Finite Element Method to compute a background solution that is locally improved by enriching the approximating space with the basis functions associated to a few meshless nodes, thus taking advantage of the flexibility ensured by the use of particles disconnected from an underlying grid. Adding the meshless particles only where needed avoids the cost of mesh refining, or even of re-meshing, without the prohibitive burden of a thoroughly meshfree approach. In particular, two enriching methods are introduced and discussed, with applications in structural mechanics.

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Simulations of turbulent Rayleigh-Bénard convection with a spectral element method

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In this study, we present direct numerical simulations of Rayleigh-Bénard convection in a rotating cylinder, comparing a finite volume approach with a spectral element method. The skew-symmetric finite volume method by Verzicco and Orlandi [4] is widely used for simulations of Rayleigh-Bénard convection in cylindrical domains. This method is second-order accurate in space. The spectral-element method offers higher-order discretizations by increasing the polynomial order of the basis functions. In theory, higher-order discretizations should produce better resolved solutions for the same number of grid points. A recent study by Scheel et al. [3] suggests that the spectral element method is indeed effective in resolving the fine scales of turbulent convection. Through a direct comparison of turbulent high Rayleigh number flows, results at a range of spatial resolutions and polynomial orders will be compared for accuracy and efficiency.

As a specific application, we address the theory by Grossmann and Lohse [2], which describes how heat transfer scales with the Rayleigh number in Rayleigh-Bénard convection. These scaling laws do not apply for the rotating case. The purpose of our simulations is to measure the heat transfer of Rayleigh-Bénard convection in a rotating cylinder, and to analyze the scaling of heat transfer under influence of rotation. We use the spectral element method implemented in the open-source code *Nek5000*, which has been developed originally by Fischer [1].

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A fully meshless method for 'gas - evaporating droplet' flow modelling

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Dilute two-phase flows are usually modelled using the Eulerian-Lagrangian approach. However, meshless Lagrangian techniques for fluid flow (gas or liquid without admixture) simulations have been actively developed during the last years [1]. These methods make it possible to develop fully meshless methods for two-phase flows as well. In [2] a method combining the viscous-vortex and the Fully Lagrangian [3] approaches was suggested to simulate particle-laden flows for which accurate calculations of the particle number density are required.

In the present study, the viscous-vortex method is developed to model two-phase flows with phase transitions. The method is based on consideration of three systems: viscous-vortex blobs, thermal-blobs and droplets; and can be applied for numerical simulation of 2D non-isothermal flows of 'gas-evaporating droplets' in the framework of the one-way coupled two-fluid approach. The carrier phase is viscous incompressible gas. The dispersed phase is presented by a cloud of identical spherical droplets. Due to evaporation, radii and masses of droplets are time dependent. The carrier phase parameters are calculated using the viscous-vortex and thermal-blob method; the dispersed phase parameters are calculated using the Lagrangian approach. The developed method retains the advantages of the Lagrangian approaches (time efficient, meshless simulations) and takes into account phase transitions in two-phase flows. A simplified model of phase transition is used, more advanced evaporation models are discussed in e.g. [4] and will be included in further studies. Two applications have been considered: (i) a standard benchmark – Lamb vortex; (ii) a cold spray injected into a hot quiescent gas. In the latter problem three cases corresponding to three droplet sizes were investigated. The smallest droplets (of the three cases considered) are shown to be easier entrained by the carrier phase and form ring-like structures. Larger droplets are shown to evaporate slowly as expected. The medium sized droplets tend to concentrate in two narrow bands stretched along the jet axis. The largest droplets form a two-phase jet, which remains close to the jet axis.

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The Qualitative Analysis and the Critical Hypersurfaces of Stationary Elliptic PDEs

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Many boundary value problems of PDEs of the applied mathematics lead to the solving of equivalent stationary elliptic quadratic algebraic equations (QAEs) with variable coefficients. The qualitative analysis of such a QAE is started here by the determination of its behavior by systematical variation of its free and linear terms, from $-\infty$ to $+\infty$ and by its visualization. It comes out that, for these variations of their coefficients, the QAE has a critical hypersurface, which is obtained by cancellation of its great determinant as in [1,2]. This critical hypersurface can be considered as a limit of existence of real solutions of the stationary elliptic QAEs.

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