MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Tagungsbericht 17/2000

Gitterlose Diskretisierungen für partielle Differentialgleichungen

16.04. - 22.04.2000

This meeting was organized by Ivo M. Babuška (Austin, USA), Michael Griebel (Bonn, Germany) and Harry Yserentant (Tübingen, Germany).

Gridless discretization methods for the solution of partial differential equations recently attracted much attention in the engineering community as well as in physics and often form a promising alternative to classical discretization schemes like finite elements or finite volumes. There are many different reasons for this development. One of these reasons is that gridless discretizations are often much better suited to scope with the problems arising from free surfaces and changes in the topology of the domain under consideration than classical methods, another reason is that the large expense for the generation and administration of the meshes and their adaptation to singularities is avoided. Meanwhile there exist many different such approaches, ranging from partition of unity finite element methods based on a Galerkin principle to pure particle methods for transport equations cleverly imitating statistical mechanics.
The aim of this conference was to bring together researchers from very different fields inside and outside mathematics to promote the exchange of ideas on this class of method and to strengthen the mathematical understanding of gridless discretizations. Many interesting discussions took place during the conference helping to establish the study of gridless discretizations as a new and interesting branch of numerical mathematics.

S. Rjasanov: Simulation of rare events by the Stochastic Weighted Particle Method for the Boltzmann equation

An extension of the stochastic weighted particle method for the numerical treatment of the Boltzmann equation has been presented. A new procedure for modeling the inflow boundary condition has been introduced and its performance has been tested in a two-dimensional example with strong density gradients. A gain factor in computing time of several order of magnitudes is achieved in specific situations.

S. Mas-Gallic: Deterministic particle methods — another way to include diffusion effects: Diffusion Velocity Method

Lagrangian methods were first introduced to solve approximately purely convective problems such as the compressible Euler equations in fluid mechanics and the Vlasov equation in plasma physics. They were rapidly found to be too narrow in their applications so that their extension to non-purely convective problems and more precisely to problems in which diffusive effects are present appeared necessary. This was first done by addition of a random walk, an easy but maybe noisy method, in which only the movement of particles is taking into account all the effects appearing in the model. Later on appeared, among other ideas, a different way to consider the particles. Their motion was no more the only way to take into account the effects contained in the model but their coefficients (weights) could also carry information (an extra degree of freedom was added). This is the basis of particle strength exchange method in which both the weight and the position of the particles cab evolve in time. In such a method, the particles are no longer considered as clouds of independent points but rather as a set of interacting ones what has permitted particle methods to tackle more general operators.
Apart form two previously mentioned methods, other methods have arisen. The diffusion-velocity method, which has been introduced by plasma physicists in the context of the Fokker-Planck equation has been presented in this talk. This method is based on the very simple idea that the diffusion of a scalar quantity ω has a preferred direction of transport, which is that of $\nabla\omega$. This remark allows a transformation of a diffusion equation into an advection equation which is non linear.

C. Lecot: On the use of quasi-random walk models for the simulation of convection-diffusion

In mathematical models that involve a combination of convective and diffusive processes the parameter that measure the relative strength of the diffusion may be quite small. So difficulties are experienced with standard numerical approximations. The method of splitting consists of reducing the original evolutionary

problem to two problems describing the convective and the diffusive processes respectively.
In this talk a particle method for solving the pure initial-value problem in s space dimensions for the convection-diffusion equations with constant diffusion coefficients has been presented. The strategy is to represent the solution at discrete times by particles. In each time interval the evolution of the system is obtained in two steps: the particles follow the convective field and the diffusion process is modeled by random walk.
The convergence of the scheme when low discrepancy sequences are used for the random walk step has been studied. The application of quasirandom numbers is not straightforward, because of correlations, and a reordering technique is used in every time step. It has been shown that an improvement in both magnitude of error and convergence rate can be achieved when quasirandom numbers are used in place of pseudorandom numbers.

D. Hähnel: Lattice Boltzmann methods

An introduction has been given in the principles of Lattice-Boltzmann methods (LBM) and their asymptotic proof for macroscopic conservation laws. Algorithmic improvements, as boundary fitting, local grid refinement and new acceleration strategies, has been reported. The flexibility of LBM has been demonstrated by examples for vortical flows, reactive flows and gas-particle flows. The developments and applications of LBM show that these methods are becoming a real alternative to classical solvers for flow problems at low Mach numbers.

R. Schaback: Radial basis functions: tools for meshless methods

This talk has focused on the essential facts of the theory of radial basis functions as needed for certain meshless methods:

- positive definite functions
- generalized interpolation and collocation
- native spaces
- error and condition analysis in the stationary and nonstationary case

Numerical examples and an outlook towards multiscale methods have been provided.

H. Wendland: Multivariate interpolation in fluid-structure interaction using radial basis functions

In the field of aeroelasticity interactions between elastic structures and fluid flows have been investigated. Since the fluid and the structural model differ in their formulation and discretization an interface model had to be introduced. In this contribution, a multivariate interpolation scheme for coupling fluid and structural models in three-dimensional space has been presented using radial basis functions. For the purpose of numerical aeroelastic computations, different basis functions have been tested: a classical global one and some smooth compactly supported radial basis functions. The scheme has been applied to a typical static aeroelastic problem, the prediction of the equilibrium of an elastic wing model in transsonic fluid flow. The resulting coupled field problem containing the fluid and the structural state equations has been solved by applying a partitioned solution procedure. The structure has been represented by finite elements and the related equations have been solved using a commercial FEM analysis code. The transsonic fluid flow has been described by the three-dimensional Euler equations, solved by an upwind scheme procedure.

A. Iske: A grid-free adaptive scheme using radial basis functions

A new grid-free adaptive advection scheme has been proposed. The method is a combination between the semi-lagrangian method and the grid-free radial basis function interpolation. Details concerning the adaptation, i.e. refinement and coarsening rules have been discussed.

M. Junk: A finite-volume particle method for conservation laws

A particle method for conservation laws has been derived based on a general partition of unity which may vary in time (moving particles). The method can be used with standard numerical flux functions. If the partition of unity is based on a finite-volume mesh, the approach reduces to usual finite-volume methods. For the one-dimensional case, a consistency analysis has been presented.

H. Yserentant: The finite mass method

The finite mass method, a new Lagrangian method for the numerical simulation of gas flow and other problems of continuum mechanics, has been presented and analyzed. In contrast to the finite volume and the finite element method, the finite mass method is founded on a discretization of mass, not of space. Mass is subdivided into small mass packets of finite extension each of which is equipped with finitely many internal degrees of freedom. These mass packets move under the influence of internal and external forces and the laws of thermodynamics and can undergo arbitrary linear deformations. Second order convergence has been proven for motions in external force and velocity fields and for the acoustic equations which result from a linearization of the Euler equations around a constant state. For the full Euler and Navier–Stokes equations, limits exist which satisfy the basic physical principles underlying these equations and can, in this sense, be regarded as solutions of these equations.

P. Leinen: The realization of the finite mass method

In contrast to finite volume or finite element methods for simulating gas flows, the finite mass method is based on a subdivision of mass into small mass packets and not on a subdivision of space into little cells. The right-hand sides of the differential equations governing the motion of the particles arise from a variational principle and are integrals which cannot be evaluated exactly. In the talk, a lagrangian discretization of these integrals has been presented that maintains the invariance and conservation properties of the method. It has been shown how the method can efficiently be implemented on a computer and how it can be parallelized both on shared and distributed memory machines. Computational experiments demonstrate that the method is very promising.

C. Gauger: Restarts in the finite mass method

The basic idea of the finite mass method as presented in the talk of Harry Yserentant is to subdivide the mass into little mass packets. Due to the fact that these mass packets can be deformed by the flow and can undergo arbitrary linear deformations, the method is second order accurate. When these mass packets deteriorate, the method has to be restarted. Fields like mass density or velocity have then to be represented by a new set of particles of regular shape. In the talk, it has been discussed how this goal can be reached. We use a total variation diminishing technique for scalar fields like mass density and local least-square approximants for the velocity. It has been shown how the amount of work and storage can be reduced by adapting the initial size of the particles to the local behavior of the flow.

M. Melenk: The Partition-of-Unity Method

The foundations of the Partition-of-Unity Method (PUM), or Generalized FEM (see the talk by I. Babuška) have been presented. This method allows for the generation of shape functions that have prescribed local behavior. The performance of the method has been illustrated by an application to the Helmholtz equation at high wave number. For additional applications and the discussion of several implementational issues, it is referred to the talk by I. Babuška.
The PUM is based on shape functions φ_i that reproduce polynomials of degree 0. An approximation result in the case when polynomials of degree $p \geq 0$ are reproduced is presented:
Theorem: Let (φ_i) be a partition of unity supported by patches $\Omega_i = \operatorname{supp} \varphi_i$. Denote $h_i := \operatorname{diam} \Omega_i$. For each i let $x_i \in \Omega_i$. Assume that

(i) $\|\varphi_i\|_{L^\infty(\Omega)} + h_i \|\nabla \varphi_i\|_{L^\infty(\Omega)} \leq c_1$;

(ii) the patches are locally comparable in size: $c_2 h_i \leq h_j \leq c_3 h_i$ if $\Omega_i \cap \Omega_j \neq \emptyset$;

(iii) overlap condition: for all i there holds card $\{j \mid \Omega_i \cap \Omega_j \neq \emptyset\} \leq c_4$;

(iv) if $x_i \in \Omega_j$, then dist $(x_i, \partial\Omega_j) \geq c_5 h_j$;

(v) for all polynomial Π of degree $p \geq 0$ there holds $\Pi(x) = \sum_i \varphi_i(x) P(x_i)$.

Under these assumptions there exists, for $k > 1$, a constant $C > 0$ s.t. for $V_{PU} = \text{span}\{\varphi_i\}$

$$\inf_{v \in V_{PU}} \|u - v\|^2_{L^2(\Omega_i)} + h_i^2 \|\nabla u - v\|^2_{L^2(\Omega_i)} \leq C h^{2\min\{k,p+1\}} \|u\|^2_{H^k(\Omega)}$$

The result can be extended to the case of hp-cloud approximation of Duarte and Oden.

I.M. Babuška: The problem of the shape function selection in the generalized finite element method

The talk has presented the main ideas of generalized method as a general case of the p-version of FEM with emphasis on the selection of the shape functions. The notion of the n-width and optimal shape functions plays an important role in the selection of robust shape functions.
Application to the elasticity equations with heterogeneous material as well as lattice material has been presented.

M. Schweizer: Parallel Partition of Unity methods for PDEs (joint work with Michael Griebel)

This talk has presented a generalized partition of unity method for parabolic, hyperbolic or elliptic PDE's based on operator splitting and the method of characteristics. The numerical results presented show that this method achieves the same convergence rates on quasirandom point sequences as FEM on uniform meshes. This holds as well for the h-version as the p-version of this method (as is also known from theory). The parallelization of this method is based on adaptive parallel trees using hashing and space filling curves for dynamic load balancing. Results for 2D/3D elliptic, hyperbolic and parabolic problems with up to 400 000 DOF's running on 1024 Processors of ASCI Blue-Pacific have been presented.

K.P. Hadeler: Dynamical models for granular media

Following the ideas of the so-called BCRF model for the slow precipitation of granular matter without internal effects, a model in the form of two coupled partial differential equations for the standing layer u and the rolling layer v has been presented (joint work with Christina Kuttler). These equations have been considered in some standard geometries (table, silo, etc.). Stationary solutions of the table problem are closely related to the eikonal equation, the distance function (of the domain) and its singular sets. Similarity solutions for the silo problem can be obtained via classical potential theory, radial solutions for circular silos can be compared to experiment. Segregation (of several species of particles) has been modeled by a system of diffusion-convection equations (work with Joel Braun).

W. Han: Error analysis of a meshfree method

In this talk, a theoretical analysis of a meshfree method — the reproducing kernel particle method — has been provided. Rigorously error estimates for meshfree interpolants and meshfree solutions, both for smooth problems and singular problems have been derived. Numerical examples have been presented confirming the theoretical predictions.

W.K. Liu: Meshless multi-scale analysis (joint work with Shaofan Li, Northwestern University)

In this presentation, the definition of multi-scale analysis has been given. The multi-resolution analysis, based on wavelet theory, has been reviewed. A meshfree multi-scale wavelet analysis has then been presented. This class of wavelets form at most a frame and they do not constitute a set of basis because of the partition of nullity. The conditioning of the resulting meshfree multi-scale system and its imposition of essential boundary condition via a bridging scale enrichment have then been presented and discussed. Applications of shear bound localization problems via wavelet adaptivity and dynamic shear bound propagation and crack initiation have been given.

A. Caglar: Smoothed-Particle-Hydrodynamics Method of higher order (joint work with Michael Griebel)

This talk has presented a new derivation of the Smoothed-Particle-Hydrodynamics method (SPH). It turns out that the method is a discretization of a convolution of the considered unknowns with the Dirac delta distribution. This approach goes back to di Lisio and Pulvirenti. They could show convergence of the method in the weak-star topology of measures. To get consistency however, one has to improve the reproducing order of the smoothing kernel, which is an approximation to the Dirac distribution. Here a variant of W.K. Liu's RKPM-Method has been presented, which is implemented by the authors. Furthermore their TREESPH approach has been presented. This method is able to deal with complex applications in astrophysics. An adaptive hash-based implementation is applied to resolve the particle densities. The parallelization is done with space-filling Hilbert curves. The method evaluates the SPH-interaction and gravitational Coulomb forces up to 64 mio. particles without cut-off. The speedup shows a parallel efficiency about 90% and the method have a good scale-up up to 512 processors on the T3E in Forschungszentrum Jülich.

J.P. Vila: SPH schemes, consistency and stability, relationship with MLS

This talk has introduced basic principle for designing of SPH like particle schemes for conservation laws. The main recipe is the use of a suitable weak discrete formulation which copes easily with consistency. Some applications in physical and industrial areas have been presented. Problems related to consistency are solved by using a renormalized formulation which use exact reproduction of derivatives of P1 polynomials. Efficient conditions for stability and consistency for the new method have been established. They also apply to MLS based schemes. A model problem of linear conservation law has been used to develop in a simpler way all these technics.

T. Sonar: Meshless collocation methods for hyperbolic conservation laws

It was reported on results concerning meshless methods for hyperbolic conservation laws. Attempts to use modified equations of established finite difference schemes encountered subtile problems with the artificial dissipation model. Using additional edge points and employing Riemann solvers lead to stable schemes with which even solutions to the compressible Euler equations can be computed. However, the degree of irregularity of the discretization points is not allowed to be large. Now difference schemes on graphs are considered which exploit certain super-approximation properties of finite differences.

C. Gaspar: A grid-free method based on the multi-level biharmonic interpolation and some applications

The presented method is based on a special scattered data interpolation technique. Instead of the explicit use of some radial basis functions (which is a popular solution tool of this problem), the interpolation function is sought as a solution of a higher order partial differential equation e.g. the biharmonic or bi-Helmholtz equation. This results in an interpolation which is similar to that of the method of radial basis functions based on the fundamental solution of the applied partial differential equation. The scattered data interpolation problem is thus converted to the solution of a biharmonic (bi-Helmholtz) equation. Using a multi-level solution technique based on the quadtree/octtree subdivision, this problem can be solved by a moderate amount of operations. Moreover, the use of large and full matrices is avoided (which is a serious drawback of the method of globally supported radial basis functions). The method does not require any spatial discretization: this is performed automatically by the quadtree/octtree algorithm, independently of the original problem which the scattered data interpolation was applied to. As it has been shown, this interpolation method generates grid-free solvers for some elliptic equations and can be applied also in the boundary element method.

S. Luding: Direct simulation of the balance equations of the hard sphere gas

Subject of this talk have been the balance equations for mass, momentum and energy for a compressible, possibly dissipative gas with internal degrees of freedom.
An ideal gas is nicely described by the kinetic theory, from which the balance equations can be derived by integration over the particle probability distribution function. Instead of solving the set of partial differential equations, the hard sphere gas is simulated directly, implying interaction laws on a "microscopic" level only. From this direct, deterministic simulation of the hard-sphere gas, one can determine each single term in the balance equations including the equation of state or other transport coefficients like viscosity. Several examples have been shown, including shock fronts and anisotropic systems.
The approach can be extended easily to account for internal degrees of freedom of the particles, energy dissipation and also energy input. The most tempting effect of dissipation is a density instability due to the loss of 'relative' kinetic energy in each collision: An initially homogeneous system evolves towards a "clustered" state, where all particles are concentrated in the so-called clusters which are separated by almost empty regions.
From the simulations, one can also extract the probability distribution functions and decide about the validity of assumptions and concepts used to simplify and to solve the underlying equations. More specific, the range of validity of the molecular chaos has been discussed.

R. Klein: Vortex element methods for slender vortices

The dynamics of slender vortex filaments in three space dimensions is important for many technological applications. A prominent example are the trailing vortices behind large aircraft (with can severely endanger smaller aircraft that try to land or start in the wake) and the helical edge vortices shed from the ends of helicopter rotor blades. The core size of such vortices is typically some orders of magnitude smaller than other characteristic system dimensions. This leads to a number of difficulties for numerical simulations: 1) Extreme resolution requirements necessitating some dynamic adaptivity or lagrangian vortex tracking. 2) Temporal stiffness due to extremely high circumferential velocities in the filament core. 3) Subtle influence of the core vorticity distribution on the overall vortex filament motion.
This presentation has described a numerical vortex element method that has been modified to overcome all of the above issues by explicit implementation of the results of slender vortex asymptotics. The developments have been carried out in joint work with Omar M. Knio, Mechanical Engineering, Johns Hopkins University, Baltimore, USA and Lu Ting, Courant Institute of Mathematical Science, New York University, New York, NY, USA.

C.D. Munz: Enforcing Gauß' law in an electromagnetic particle-in-cell scheme

Beside hyperbolic evolution equations the Maxwell-Vlasov equations also contain divergence constraints for the electric and magnetic fields. Due to approximation errors that appear in the numerical treatment of the motion of the charged particles, charge conservation errors may appear. It is shown that this may lead to errors in the divergence condition for the electric field, usually called Gauß' law, which may increase in time and falsify the numerical solution. This can be avoided by coupling the evolution equations with the divergence constraints. Such a constrained formulation of the Maxwell equations has been introduced. Numerical results for a simple model problem have been shown.

C. Lubich: Exponential Integrators for Time Discretization

The exponential of the Jacobian, or related matrix functions, can be successfully used in devising integration schemes for stiff or oscillatory differential equations. Though such methods can be traced back to the 1950's and 60's, they have only recently become attractive through the approximation of the product of the matrix exponential with a vector by Krylov subspace methods. This approximation converges superlinearly and — unless a good preconditioner is available — is superior to iterative methods for the corresponding linear systems in implicit integration methods. Another interesting aspect of exponential integrators is that they offer the possibility to accurately approximate near-harmonic oscillations, avoiding the time step restrictions of standard integrators. Tailor-made exponential integrators can be devised for equations with a special structure. As examples, an integrator for the Finite Mass Method of Yserentant et al. has been presented, which copes with the stiffness arising from viscous forces and friction terms; and a Gautschi-type integrator for oscillatory equations of the type of semilinear wave equations.

H. Riffert: Relativistic Smoothed Particle Hydrodynamics (SPH)

The development of numerical methods for relativistic flows is strongly motivated by astrophysical applications, such as high-velocity jets in radio galaxies or accretion flows around massive black holes in the centers of active galaxies. The starting point of our approach is the $(3+1)$ decomposition of space-time according to Arnowitt, Deser and Misner (1961). With a proper definition of a density and 3-velocity it is possible to convert the equation of continuity into a form that is formally identical to the non-relativistic equation. From that one can find corresponding momentum- and energy-flux variables such that for non-viscid flows a set of Lagrangian hydrodynamic equations is obtained which strongly resemble their non-relativistic counterparts. Thus, the standard SPH-method including standard kernels is used to discretize these equations. The method has been tested with the 1D-shock-tube problem, a 1D wall-shock calculation, and a 2D jet streaming into a low-density medium. Shocks are resolved by a relativistic version of the artificial viscosity. As a result, it is possible to simulate flows with shocks up to Lorentz-factors of at least 1000. The method derived so far cannot be applied directly to viscous flows because the viscous forces contain 2nd order time derivatives of the velocity which cannot be transformed away because of the parabolic nature of the corresponding operator. Different methods have to be developed for this case.

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