INSTITUT FüR ANALYSIS UND NUMERIK

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1. Leitung

Prof. Dr. Hans-Christoph Grunau
Prof. Dr. Lutz Tobiska (Geschäftsführender Leiter)
Prof. Dr. Gerald Warnecke
Priv.-Doz. Dr. Bernd Rummler

2. Hochschullehrer

Prof. Dr. Klaus Deckelnick
Prof. em. Dr. Herbert Goering
Prof. Dr. Hans-Christoph Grunau
Priv.-Doz. Dr. Matthias Kunik
Priv.-Doz. Dr. Bernd Rummler
apl. Prof. Dr. Friedhelm Schieweck
Prof. Dr. Lutz Tobiska
Prof. Dr. Guofang Wang
Prof. Dr. Gerald Warnecke

3. Forschungsprofil

AG Analysis (Numerische Analysis: Tobiska, Schieweck)

- Konvergenz, Stabilität und Genauigkeit von Finite Elemente Methoden für nichtlineare partielle Differentialgleichungssysteme, insbesondere in der numerischen Strömungssimulation
- Eigenschaften der Lösung singulär gestörter Probleme
- A posteriori Fehlerschätzung und adaptive FEM
- Entwicklung effektiver Algorithmen zur Lösung hochdimensionaler Gleichungssysteme auf modernen Rechnerarchitekturen
- Finite Elemente Methoden zur Lösung der Navier-Stokes-Gleichungen in Gebieten mit freiem Rand und Entwicklung geeigneter Mehrgitterlöser

AG Analysis (Nichtlineare partielle Differentialgleichungen: Deckelnick, Grunau, Rummler, Wang)

- Nichtlineare elliptische Probleme:

Kritisches Wachstum, Bezüge zur reellen und komplexen Differentialgeometrie sowie zur Mechanik

- Nichtlineare Evolutionsgleichungen:

Bezüge zur reellen und komplexen Differentialgeometrie, nichtlineare Dynamik

- Gleichungen der Hydrodynamik
- Eigenwertprobleme
- Freie Randwertprobleme
- Nichtlineare Funktionalanalysis

- Hydrodynamik (Navier-Stokes-Gleichungen)
- Nichtlineare elliptische Randwertprobleme, Bezüge zur Mechanik
- Analytische Untersuchung qualitativer Eigenschaften von Lösungen
- Nichtlineare partielle Differentialgleichungen (Existenz, Regularität und Einzigkeit von Lösungen)
- Eigenfunktionen des Stokes Operators (explizite Darstellungen, Vollständigkeit)
- Nichtlineare Funktionenanalysis (Operator-Kommutatoren, pseudomonotone Operatoren)
- Laminar-turbulentes Umschlagsverhalten inkompressibler Strömungen in speziellen Gebieten (direkte numerische Simulation, Bifukationsmethoden)
- Geometrische Evolutionsgleichungen: Existenz, Eindeutigkeit und Eigenschaften von Lösungen; Konvergenzanalyse numerischer Näherungsverfahren
- Freie Randwertprobleme
- Navier-Stokes-Gleichungen (Stabilität kompressibler Strömungen; Kontrolltheorie für inkompressible Strömungen)
- Vollständig nichtlineare Gleichungen aus der konformen Geometrie
- Sasaki-Ricci-Fluss und Sasaki-Einstein Mannigfaltigkeiten

AG Numerische Mathematik (Warnecke, Kunik)

- Konvergenz, Stabilität und Genauigkeit von Diskretisierungsverfahren (FEM, FVM, FDM, kinetische Verfahren) für partielle Differentialgleichungssysteme, Entwicklung numerischer Verfahren
- Theoretische und numerische Untersuchung von Systemen von Erhaltungsgleichungen, insbesondere in der Gasdynamik, Mehrphasengemische, laserinduzierte Gasblasen
- Numerische Methoden für Populationsbilanzgleichungen in der Verfahrenstechnik und der Bioverfahrenstechnik

4. Forschungsprojekte

Projektleiter: Prof. Dr. Klaus Deckelnick

Kooperationen: Michael Hinze, Hamburg

Förderer: DFG; 01.10.2009 - 30.09.2012

Galerkin-Verfahren fuer Kontrollprobleme mit partiellen Differentialgleichungen

Das Projekt befasst sich mit der Entwicklung und Analyse von Diskretisierungen von Optimalsteuerungsproblemen, in denen die Zustandsgleichungen durch parabolische partielle Differentialgleichungen gegeben sind.

Projektleiter: Prof. Dr. Hans-Christoph Grunau

Projektbearbeiter: Dr. Anna Dall Acqua; Prof. Dr. Klaus Deckelnick; apl. Prof. Dr. Friedhelm Schieweck

Kooperationen: PD Dr. Steffen Fröhlich (FU Berlin)

Förderer: DFG; 01.10.2008 - 30.09.2010

Randwertprobleme für Willmoreflächen - Analysis, Numerik und numerische Analysis

Die Willmoregleichung, d.h. die Euler-Lagrange-Gleichung zum Willmorefunktional, zählt zu den wichtigen und anspruchsvollen Herausforderungen der nichtlinearen Analysis: Sie ist quasilinear und von vierter Ordnung; viele aus der Theorie von Gleichungen und Systemen zweiter Ordnung her wohlbekannten Methoden versagen zu einem großen Teil. Dennoch konnten in letzter Zeit einige bemerkenswerte Fortschritte u.a. von L. Simon, E. Kuwert, R. Schätzle, T. Riviere u.a. erzielt werden. Bislang wurde das Willmorefunktional meist nur auf unberandeten kompakten Mannigfaltigkeiten studiert, da hier großer Gewinn aus globalen differentialgeometrischen Eigenschaften gezogen werden konnte. Hinsichtlich Randwertproblemen liegen erst ganz wenige Resultate vor: Die ohnehin schwierige Gewinnung von Kompaktheit / Abschätzungen wird hier nochmals komplizierter. Wir wollen mit numerischen Studien und analytischen Untersuchungen von Randwertproblemen in symmetrischen Prototypsituationen beginnen und damit eine Richtung aufzeigen, unter welchen Bedingungen zu erwarten sein wird, mit a-priori-beschränkten Minimalfolgen arbeiten und a-priori-beschränkte klassische Lösungen erhalten zu können. Darüber hinaus sollen numerische Algorithmen und Konvergenzsätze in allgemeineren Situation entwickelt werden, z.B. für Graphen über zweidimensionalen Gebieten. Diesbezügliche Ergebnisse könnten Entwicklungen hin zu parametrisch beschriebenen

Flächen vorbereiten. Im vorliegenden Projekt werden Analysis, numerische Analysis und Numerik gleichberechtigt und eng miteinander verzahnt bearbeitet. Die Analysis profitiert von den numerischen Studien, während die Numerik ganz wesentlich auf die analytischen Vorarbeiten aufbaut. Die numerische Analysis schlie\ss lich setzt sowohl auf den numerischen als auch den analytischen Vorarbeiten auf und wirkt umgekehrt hierauf zurück.

Projektleiter: Prof. Dr. Lutz Tobiska

Projektbearbeiter: Sergey Beresnev

Kooperationen: Prof. Dr. V. Polevikov (Minsk, Belarus)

Förderer: DAAD; 17.12.2007 - 17.12.2011

Einfluß der Verteilung ferromagnetischer Teilchen auf die Oberflächenform magnetischer Fluide

Bei der numerischen Simulation freier Oberflächen magnetischer Fluide wurde bislang vorausgesetzt, dass die ferromagnetischen Teilchen in der Flüssigkeit gleichverteilt sind. Diese Annahme ist jedoch innerhalb von Magnetfeldern mit starken Gradienten nicht gegeben. Ziel des Projektes ist es, an ausgewählten Beispielen den Effekt der Teilchendiffusion auf die Gestalt der freien Oberfläche zu studieren.

Projektleiter: Prof. Dr. Lutz Tobiska

Projektbearbeiter: Dr. S. Ganesan, Dr. H. Xie

Kooperationen: Prof. Dr. Hackbusch (MPI Leipzig), Prof. Dr. John (Uni Saarbrücken), Prof. Dr. K. Sundmacher, Prof. Dr. Kienle

Förderer: Bund; 01.07.2007 - 30.06.2010

Gekoppelte Simulation von Partikelpopulationen in turbulenten Strömungen

Im Verbundsprojekt werden neue Methoden der angewandten Mathematik zur Behandlung gekoppelter Populationsbilanzen in Strömungsfeldern entwickelt und zur modellgestützten Analyse und Führung eines industriellen Kristallisationsprozesses genutzt. Die Ergebnisse der mathematischen Methodenentwicklung und deren Übertragung auf den industriellen Prozeß sollen über die Know-How-Transfer-Kette der Verbundpartner zur Analyse und Verbesserung von partikelbildenden strömungssensitiven Verfahrensprozessen eingesetzt werden.

Projektleiter: Prof. Dr. Lutz Tobiska

Projektbearbeiter: Dipl.-Math. Sangeetha Rajasekaran

Förderer: DFG; 01.08.2006 - 28.02.2010

Hochauflösende numerische Verfahren für dynamische Zweiphasensysteme mit Surfactants

In vielen zweiphasigen Prozessen spielen grenzflächenaktive Substanzen wie z. B. Tenside, sogenannte Surfactants (surface active agents), eine wesentliche Rolle. Diese lagern sich an der Grenzfläche eines Fluids an und verändern seine Grenzflächenspannung. Dadurch entstehen die Marangoni-Kräfte, die zu einem veränderten Strömungsverhalten nahe der Grenzfläche führen. Ziel des Projektes ist die Entwicklung, Analyse und Implementation hochauflösender numerischer Verfahren, um die Dynamik der sich wechselseitig beeinflussenden Prozesse besser verstehen zu können. Die Modellierung basiert auf den inkompressiblen Navier-Stokes Gleichungen für beide Phasen, je einer zusätzlichen Bilanz für die Konzentration des Surfactants in den Kernphasen und auf der Grenzfläche, einer thermodynamischen Gleichgewichtsbeziehung und einem Gesetz, das die Abhängigkeit der Grenzflächenspannung von der Grenzflächenkonzentration des Surfactants beschreibt. Numerisch erfordert die Bilanz der oberflächenaktiven Substanzen - mathematisch gesehen eine dynamische Randbedingung - eine sehr genaue Auflösung der dynamisch bewegten Grenzfläche, die durch isoparametrische finite Elemente höherer Ordnung und eine ALE-(Arbitrary-Langrangian-Eulerian)-Formulierung der Gleichungen in den Kernbereichen erzielt werden soll.

Projektleiter: Prof. Dr. Lutz Tobiska

Projektbearbeiter: Dipl.-Math. Stephan Schütze

Kooperationen: Dr. P. Knobloch, Associate Prof. (Faculty of Mathematics and Physics, Charles University Praha)

Förderer: DFG; 01.04.2007 - 31.05.2010

Numerical simulation of the interactions between a ferrofluid and an immersed permanent magnet

This project is devoted to the numerical modelling of interactions between a ferrofluid with a free surface and a permanent magnet immersed in this ferrofluid.

It is a highly nonlinear problem involving the numerical simulation of magnetic fields, incompressible fluid flow and rigid body motion. All these components influence each other and both the position of the rigid bodies and the form of the domain occupied by the ferrofluid are generally not known in advance.

The goal is to develop robust, accurate and efficient solvers for problems of the mentioned type. This will include research on linearization strategies, time stepping techniques, discretization concepts and efficent solvers for the arising large sparse systems of linear equations. In addition, appropriate tools for handling the moving boundaries have to be developed.

Projektleiter: Prof. Dr. Guofang Wang

Förderer: DFG; 31.05.2007 - 31.05.2009

Analytic aspects of almost Kaehler manifolds

This project deals with compatible metrics on symplectic manifolds, whose Ricci tensor ommutes with its compatible almost complex structure and whose Hermitian scalar curvature is constant. We want t to understand analytic and geometric aspects of such compatible metrics and hope to have applications in the direction of classifying symplectic manifolds, especially, in the 4-dimensional case.

Projektleiter: Prof. Dr. Gerald Warnecke

Projektbearbeiter: Narni Nageswara Rao

Kooperationen: Dr. Jitendra Kumar - IAN, Dr.-Ing. Mirko Peglow-FVST, Jun.-Prof. Dr.-Ing. Stefan Heinrich - FVST, Prof. Dr. Evangelos Tsotsas - FVST, Prof. Dr.-Ing. Dr. h.c. Lothar Mörl - FVST

Förderer: DFG; 01.10.2005 - 31.01.2009

GRK Mikro-Makro-Wechselwirkungen in strukturierten Medien und Partikelsystemen "Population Balance Modelling by the Discrete Element Method (DEM) in Fluidized Bed Spray Granulation"

In a fluidized bed, particle growth is governed by different mechanisms; granulation, coating agglomeration, attrition and breakage. The agglomeration of particles is a process in which particles collide and stick together to form new large particles. This process is described by population balance equations for a time dependent particle size distribution function. The decisive quantities determining the process are integral kernels describing the collision frequency and intensity, adhesion probability and agglomeration rate. The aim of this project was to simulate these quantities using the Discrete Element Method (DEM). From these microscopic simulations the kernels werel be derived by averaging to a coarser scale. The project was completed with doctoral thesis of N.N. Rao.

Projektleiter: Prof. Dr. Gerald Warnecke

Projektbearbeiter: Rajesh Kumar

Kooperationen: Dr. Jitendra Kumar - IAN, Dr.-Ing. Mirko Peglow-FVST, Prof. Dr. Evangelos Tsotsas - FVST

Förderer: DFG; 01.08.2007 - 30.07.2010

GRK-Mikro-Makro-Wechselwirkungen in strukturierten Medien und Partikelsystemen "Numerical methods for population balance equations with high property space dimension"

The topic of this project is the numerical analysis and computation of population balance equations (PBEs). Aggregation and breakage PBEs can be rewritten in mass conservative form whereas growth is number conserving. Therefore, one of our aims is to achieve the coupling of all the particulate processes in such a way that both number and mass are preserved. We investigated mathematically and verified numerically schemes which are both number and mass preserving for the coupled processes. The second aim is to study the existence of approximated solution using the finite volume scheme for binary aggregation and general breakage problem. Further, we explored the stability and the convergence analysis of the method for non-linear aggregation and linear breakage problem. This is an extension of the results given by J.P. Bourgade and F. Filbet. Moreover, we also study the two-dimensional problems by using sectional methods such as the cell average and the fixed pivot techniques.

Projektleiter: Prof. Dr. Gerald Warnecke

Projektbearbeiter: M.Sc. Carlos Cueto Camejo

Förderer: Sonstige; 01.08.2009 - 30.07.2012

Biological population balance equations with non-local behavior and related Hamilton-Jacobi equations

We study models for adaptive dynamics of populations in biology that carry specific traits. In recent years models have been derived that we wish to study analytically and numerically. These are population balance equations with nonlocal terms. Asymptotic consideration lead to related Hamilton-Jacobi equations.

Projektleiter: Prof. Dr. Gerald Warnecke

Kooperationen: B.-W. Schulze, Potsdam, Chen Shuxing - Shanghai, Prof. Dr Chen Hua - Wuhan University China

Förderer: DFG; 01.04.2004 - 31.03.2009

Folgeprojekt "Partial Differential Equations and Applications in Geometry and Physics"

The mathematical theory of systems of time-dependent nonlinear hyperbolic and mixed type partial differential equations, more specifically conservation laws, in more than one space dimension is in a very unsatisfactory state. The basic issue of global in time existence of solutions is still an open problem. Since the 1950s the existence and uniqueness for scalar equations was solved in the seminal work of Oleinik and Kruzkov. For systems in one space dimension there is an existence theorem of Glimm for data with small total variation since 1965. The small data requirement was only relaxed for some 2×2 systems by DiPerna in the early eighties. Uniqueness is not completely understood, even in the one-dimensional case, despite some recent progress by Bressan, T.-P.\ Liu and T.\ Yang. This field offers a wealth of open problems for future research. Shock waves are discontinuous weak solutions of the equations. This generalization of solutions in the sense of distributions leads to a serious non-uniqueness problem which necessitates the use of additional so-called entropy conditions in order to select the physically meaningful solutions. Any approximation has to be checked whether it leads to these meaningful solutions. Wang Jinghua (Beijing) and Warnecke (Magdeburg) started their collaboration by partially proving the entropy consistency of large time step schemes. Later the convergence of finite difference approximations for relaxation systems and the Ruijgrok-Wu model in kinetic theory were proven. Also results on convergence rates and error estimates were achieved, some jointly with Wang"s former student Liu H. Traveling wave solutions for conservation laws with viscous and dispersive perturbations are smooth approximations of shock waves. The existence and stability of solutions that are perturbations of such traveling waves was proven by Pan Jun, Chinese doctoral student of Warnecke (Magdeburg).

Projektleiter: Prof. Dr. Gerald Warnecke

Projektbearbeiter: M.Sc. Ee Han

Förderer: Sonstige; 01.06.2009 - 31.05.2012

International Max Planck Research School for Analysis, Design and Optimization in Chemical and Biochemical Process Engineering Magdeburg "Analytical and numerical analysis of two phase flow"

Two phase flow, as a particular example of multiphase flow which occur commonly in nature, is an interesting and challenging field in mathematical and fluid mechanics. Since the two phase flows are characterized by interfaces, the central problem in the theory of two phase flow is the treatment of interfaces. Historically, the most straight forward model approach two phase flow is the interface model, which treats flow boundaries as a free boundary in the flow. Probably in most cases, it is not necessary and hard to get a detailed knowledge of the position of the interfaces. Therefore homogenized or averaged mixture models are a better alternative to the interface model described above. In particular for dispersed flows with a large number of droplets, bubbles or particles. In our project, we are mainly concerned with the second kind of model, which includes two continuity, two momentum, and two energy equations for both phases. The averaging of the single phase equation results in additional interaction term, which described the interaction between two systems. The generical model is a system of nonconservative hyperbolic equations. Several features make the study attractive

1. The nonconservative derivative makes the mathematical structure much more complicated than the conservative laws. How to deal with this nonconservative part is still a problem in analysis and numerical investigations.
2. The eigenvalues of the generic systems are not ordered, if two eigenvalues meet each other, the resonance phenomenon will happen. This is a open problem.
3. The well known Euler equation in a duct variable cross-section has been studied by many persons as a resonance system. Here we would like to get insight for the complete solution of the Riemann problem for the Euler equation in a duct variable cross-section, then construct a Godunov-type scheme based on afore mentioned mathematical analysis. In the end we hope to gain deeper understanding for the generical model by considering the Euler equation in a duct variable cross-section as a submodel of the generic model.

Projektleiter: Prof. Dr. Gerald Warnecke

Projektbearbeiter: MSc. Ali Zein

Kooperationen: Frank Duderstadt (WIAS, Berlin), Wolfgang Dreyer (WIAS, Berlin)

Förderer: DAAD; 20.09.2007 - 20.09.2010

Numerical methods for multi-phase mixture conservation laws with phase transition

Multi-phase mixtures occur very commonly in nature and technology. Several mathematical models have been developed to describe the flow of such mixtures. But both the mathematical modelling and numerical computation of multi-phase flows are associated with certain difficulties. The difficulties is modelling concern the physical transfer processes taking places across the interface such as mass, momentum and heat transfer, and phase change. By using averaging technique of the single phase equations results additional terms, which describe those transfer processes. The exact expressions for the transfer terms are usually unknown. Also there appear differential terms that are extracted from the transfer terms that prevent the system from being in divergence form. Therefore, they are referred to as the non-conservative terms. The numerical difficulties arise the resulting model cannot be written in divergence form (conservative form) due to the existence of non-conservative terms. And in this case one cannot define a weak solution for the systems of governing equations in the standard sense of distributions, as it is done for the systems of conservation laws. The primary goal of this project is to improve and validate numerical schemes for the solution of two-phase flow equations concerning non-conservative terms. There exist a large number of numerical methods for conservation laws which use an exact or approximate solution of the local Riemann problem at the cell interfaces. These algorithms belong to the family of Godunov-type methods. To apply these methods to two pase flows we need to improve an efficient and robust Riemann solver for the non-conservative systems. Also we need to improve an accurate methods for the discretization of the non-conservative terms. Another problem in the numerical solution of two-phase flows occurs when pure phases are present in the domain. Then for the other phase, the situation is analogous to the occurence of vacuum in the solution of the usual fluid dynamics equations. For the Euler equations, there are two different ways to attack the problem of vacuum occurrence. One is to track the gas-vacuum interface explicitly. However in multi-D this becomes very complicated due to topological problems, like merging, breaking, and creating of the interfaces. An alternative is to admit a negligible amount of the phase, which is supposed to disappear. It is important to use a positively conservative method for the solution of the interface problems between almost pure phases. Otherwise a smallest numerical inaccuracy would lead to negative pressure or densities. We plan to study this problem more thoroughly.

Projektleiter: Prof. Dr. Gerald Warnecke

Projektbearbeiter: M.Sc. Bolaji James Adesokan

Kooperationen: Prof. Dr. Kienle

Förderer: Sonstige; 01.10.2008 - 30.09.2011

Population balance models in bio-process engineering

During vaccine production, optimal production of viruses in a biorector is desirable. Mathematical modeling of viruses becomes a natural choice to achieve this aim. In this project, a model for interaction between the Influenza A virus and its host is considered. It´s a differential equation, which does not only assume dependence on current time but also includes a time lag. Our task is to develop a robust numerical algorithm for solving the evolved delay differential equations (DDEs). Also, from the theoretical point of view many intriguing properties of the model will be treated because the delay(lag) term in the model formulation changes the classical properties of well known solutions methods for ordinary differential equation and Partial differential equations.

Projektleiter: Prof. Dr. Gerald Warnecke

Projektbearbeiter: Dr. Maren Hantke

Kooperationen: Boniface Nkonga (Bordeaux, Frankreich), Christophe Berthon (Bordeaux, Frankreich), Frank Duderstadt (WIAS, Berlin), Philippe Hekey (Strassburg, Frankreich), Rémi Abgrall (Bordeaux, Frankreich), Richard Saurel (Marseille, Frankreich), Thomas Kurz (Göttingen), Werner Lauterborn

(Göttingen), Wolfgang Dreyer (WIAS, Berlin)

Förderer: DFG; 01.01.2005 - 31.12.2009

Homogenized systems for liquid-vapour transition in unsteady compressible two-phase flow

In this project, we consider the liquid vapour flow as a homogenized mixture of the two phases. The resulting models pose a major challenge to mathematics, since there are a number of important open questions to be studied. The primary goal is to improve goal is to improve and validate numerical schemes for such models. Numerical solutions are needed in many diverse engineering applications involving phenomena such as liquid sprays of bubbly flows. In order to improve the quality of numerical results we need to address some mathematical issues concerning the modelling and resulting well-posedness of the equations. Also we will have to develop a deeper understanding of the theory and numerical methods for hyperbolic systems of equations containing non-conservative derivatives. Another challenge is phase extinction, which is related to vacuum states in gas dynamics. Further, it will be necessary to encorporate phase transitions into the models and numerical computations. Gefördert von der DFG im Rahmen der DFG-CNRS-Forschergruppe 563 "Micro-Macro Modelling and Simulation of Liquid-Vapour Flows".

Projektleiter: Prof. Dr. Gerald Warnecke

Projektbearbeiter: Ankik Kumar Giri

Kooperationen: Dr. Jitendra Kumar - IAN

Förderer: Land (Sachsen-Anhalt); 01.10.2007 - 30.09.2010

International Max Planck Research School for Analysis, Design and Optimization in Chemical and Biochemical Process Engineering Magdeburg "Mathematical Theory for the Dynamics of Coagulation-Fragmentation Equations for Process Engineering"

Coagulation fragmentation equations are time dependent integro-differential equation for the dynamics of particle property distributions. This project is concerned with the mathematical and numerical analysis of these equations. These equations are well known in various branches of engineering including nano-technology, crystallization, comminution, precipitation, polymerization, aerosol and emulsion processes. The objective of this work is to prove existence and uniqueness of solutions for large class of kernels. Furthermore, it is of great interest to investigate the gelation phenomenon, equilibrium solutions, metastability, and asymptotic behavior of solutions. A further important task is to work with multiple fragmentation problems. Several researchers analyzed mathematically binary fragmentation problems. However, a mathematical study of multiple fragmentation equations is a challenging problem. Our objective is to establish some results on existence and uniqueness for general breakage as well for coupled aggregation and breakage models. Furthermore, in this case properties of solutions like mass conservation, positivity, the shattering phenomenon etc. are also open problems.

Projektleiter: Prof. Dr. Gerald Warnecke

Projektbearbeiter: Vincent Ssemaganda

Kooperationen: Prof. Dr. A. Seidel-Morgenstern, Prof. Dr. Jitendra Kumar-IIT Kharagpur, Indien

Förderer: Land (Sachsen-Anhalt); 01.10.2007 - 30.09.2010

International Max Planck Research School for Analysis, Design and Optimization in Chemical and Biochemical Process Engineering Magdeburg "The Dynamics of the Becker-Döring System of Nucleation Theory applied in Process Engineering"

In this project we study the Becker-Döring model mathematically and numerically. This model describes nucleation process of droplets in gas, crystals in solutions or liquid droplets in a crystalline solid such as Gallium Arsenide (GaAs). It is a special case of the discrete coagulation-fragmentation equations. It has several applications including suspensions, aerosols, enantiomer crystallization etc. One of the objectives is to extend some results on existence and uniqueness of solutions. Furthermore, efficient computation of solutions through metastable phases is a big challenge due to a very large system of equations required to exhibit the metastability. Our aim is to provide a computationally efficient numerical method for solving the model. Regarding efficient computation, one possibility could be model reduction in such a way that over all balances like mass conservation and the total number of aggregates are accurate enough. The model reduction idea relies on considering computation of only a few concentrations. This leads to the inconsistency of the moments, that is, poor prediction of total aggregates and break down of mass conservation. In order to overcome inconsistency of the numerical method one can use the idea of the cell average technique which is well known for solving a general aggregation-breakage equation. This technique predicts the complete density distribution as well as the moments of the distribution very accurately by considering only a few grid points for the computation.

5. Veröffentlichungen

Originalartikel in begutachteten internationalen Zeitschriften

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