INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Smash

Simulation, Modelization and Analysis of Heterogeneous Systems in mechanical engineering

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2. Overall Objectives

SMASH is a common project between INRIA and the University of Provence. The main topic of our project focuses on problems related to both mathematical and numerical modelization of heterogeneous flows such as multiphase media, granular materials or reactive flows with mass transfer. The scientific themes in concern are the setting up and improvments of models for these flow including both definition and analysis of discretization methods and schemes for their numerical simulation. The final aim is to implement the resulting algorithms on parallel machines.

One of the main original feature of the SMASH research on that topic lies in the way we deal with multifluid flows (interface problems). We use an eulerian approach with a diffuse interface model. The two different media are not modelled separately (using adequate scheme for each phase) nor the interface needs to be defined explicitely. On the opposite, the diffuse interface zone is considered as a true multiphase region and described with a two-phase model. With such an Eulerian approach, numerical problems related to the discontinuities of the state equations through the interface which occur when using separate models for each phase, do not appear anymore.

The domains in which two-phase flows are of interest are widely spread through the industry (nuclear industry, oil company industry, car engine technology, food industry ...) but also in forest fire, biomedical engineering, detonation or astrophysics research areas.

3. Scientific Foundations

3.1. Modelization of multiphase media

Keywords: *Hamilton principle*, *Homogenization*, *mixture models*, *two-phase models*.

The microcospic description of an heterogeneous medium has to take into account the specific physical properties of each material component. For both practical and numerical reasons, it may be impossible to take into account all those microscopic features. As an illustration, one m^3 of water mist typically contains a range of about 10^8 to 10^{12} droplets! Modelizing such an heterogeneous medium consists in replacing it by an artificial mixture that ideally would have the same averaged properties. The resulting *multiphase* models are very far from the classical Euler or Navier-Stokes models.
The definition and setting of such multiphase models may be based on different techniques.
The first formalism [28], is very similar to the techniques involved in the definition of statistical models of turbulence with the use of averaging operators. It leads to an open set of equations (that is there are more unknowns than there are available equations). A way to close that system is to take into account some physical assumptions concerning the behaviour at the micro-scale level. This approach is certainly the most used in the industry but leads to difficult open questions in applied mathematics such as the hyperbolicity of the resulting models and the definition of non-conservative products. This methodology was the starting point of our studies in multiphase modelling and lead us to promote the use of two-pressure, two-velocity *hyperbolic* models.
However, with this type of modelization, closure assumptions concerning the microscale behaviour have to be formulated. This is an extremely difficult task. Therefore, we are also investigating a modelization formalism based on the Hamilton principle of least action [32]. The advantage of this formalism is that the only assumptions are on the definition of the potential energy associated to the flow.
Using either the first or the second technique results in a set of non linear partial differential equations (PDE). Then, we need to discretize it by some numerical scheme in order to get a set of algebraic equations that in turn will furnish the discrete solution. We are therefore faced to mainly two types of difficulties: the first class of difficuties consists in finding the good set of PDE's to model the multiphase flow we want to study; the second class comes from the choice of the discretization scheme.
To avoid this addition of dificulties, we have recently introduced an original modelization technique [1]. In this approach, we start with the continuous equations defined at the microscale level but instead of averaging it, we *first* discretize those microscale continuous equations *before* filtering the resulting set of discrete equations. With this technique, we end-up directly to a macroscale discrete model.

3.2. Modelization of of interface and multifluid problems

Keywords: *Diffuse interface*, *Eulerian Models*, *Front Capturing*, *Multifluid mixtures*.

An important part of CFD is to get a detailed description of the interaction between two different fluids at the scale of the interface between them. This is what we will call a *multifluid* problem. At the present time, tracking methods (and specially the level-set methods) are certainly the most used technologies to treat this problem.
"Capturing" or diffuse interface approach, where the interface is not defined explicitely as a discontinuity surface but as non-zero thickness mixing zone (where the physical quantities are continuously varying) are just begining to be used. Actually, before the original work of Abgrall [27] the capturing methods were pleagued by the difficulty of computing the pressure in the mixing zone. Abgrall shows the feasability of interface capturing methods provided that one gives up partially the conservative form of the equations. Improving upon this contribution, our project develops an original diffuse interface method where the artificial numerical

zone is considered as a true two-phase flow region. Although seemingly artificial, this permits to consider a model that can handle huge density ratio and very different thermodynamics.

This front capturing - diffuse interface technique has proven its ability of solving interface flow problems more simply than usually and moreover offers the possibility to treat not only interface problems between pure fluids but also interfaces between mixtures (as for instance the boundaries of a cloud) in the same formalism.

3.3. Approximation methods

Keywords: *Finite Volume methods*, *Low Mach Compressible flows*, *Riemann Solvers*.

All the mathematical models considered and studied in SMASH consist in either a hyperbolic or parabolic system of PDE's. The discretization techniques applied to these PDE should respect the properties of the continuous model such as conservativity, positiveness preserving (e.g. pressure, density), jump conditions, maximum principle or entropy inequality. Most of our numerical methods are based on finite volume discretizations [29]. That indeed allows us to keep the full description of the physics of the media by solving local *Riemann problems* [33] corresponding to the evolution of the medium variables through a plane interface separating two physical states. SMASH focuses its efforts into the development of approximation methods using either exact or approximate Riemann solvers.
When the resulting model is non conservative, which occurs as a "mechanical" consequence when using an averaging process, additional mathematical and numerical difficulties arise. From a theoretical point of view, the question of giving a sense to the distribution product does not admit a sensible answer since the works of Schwartz [31] and as a consequence, the numerical approximation of non-conservative terms is unclear. Our discretization methods are based on the principle which states that both velocities and pressures should remain constant through a contact discontinuity. The resulting discretization schemes respecting that principle appear to be both robust and efficient for interface flow problems compared to most of other existing methods.

Another difficulty encountered in solving two-phase flow problems comes from the high disparity between the wave speeds of each existing fluid material. In particular, one of the fluids may be very close to the incompressibility limit. In that case, we face up the problem of very low Mach number flows. The numerical treatment of these flows is still a problem and involves non trivial modifications of the original upwind schemes [3]. Our investigations in that domain concerns both acoustic and incompressible aspects in methodologies for setting suitable numerical methods.

3.4. Solution algorithms

Keywords: *Grid Computing*, *Multigrid methods*, *Multilevel methods*, *Parallelism*.

In a multigrid method [30]- [34], we need to define a series of grid levels, each of them is associated with different frequency mode intervals. Another important ingredient of these methods is the choice of a so called *smoother* which may be any classical iterative method having the property of efficiently and rapidly damping the high frequency modes of the error associated with the finest level discretization; the residual equation, written on a coarser level may therefore be approximately solved by the same smoother in the sense that high frequency modes of the coarse level error are in turn rapidly damped by that smoother. When suitably projected back to the finest level, both high frequency (considered on the fine level) and low frequency (which are also high frequency at the coarser level) modes of the original error have been damped resulting in a better approximation of the discrete exact solution. In fact, when more than two grid levels are considered, each residual equation is solved using the same smoother before being projected onto a coarser level, and so on, until reaching the coarsest level where a direct method may be used to exactly solve the coarsest residual equation. Getting the final solution consists in projecting back from coarse to fine level, combined with or without post smoothing, the corrected error until reaching the finest discretization level on which the discrete solution has to be defined. In multigrid theory, it can be shown that the complexity of these methods is proportional to the discretization node number when applied to elliptic type problems. That therefore means that the solution cost of the finest level discrete system of algebraic equations up to the order of finest level discretization error is directly proportional to the total number of degrees of freedom of that finest level.

Concerning the definition of the grid levels, we focus on construction methods based on the finest level ingredients as initial data, where the finest level discretization grid is supposed to be fully unstructured. This means that we are interested in either agglomerating or reconstruction techniques (geometrical definition of the grid levels) or algebraic techniques (the algebraic definition of the discrete coarser level residual problem is directly defined from the discrete fine level algebraic operators).

4. Application Domains

4.1. Panorama

With a large experience in working on numerical fluid mechanics problems, SMASH studies focuses its particular interests on compressible multiphase or multifuid flows; the application domains involves energy and transport industries: aeronautics, car engine combustion research, space research, oil company research, research on electricity and nuclear centers hazards, but involves also other various domains such as astrophysics and detonation studies.

4.2. Transport industry

Aeronautics The main needs in that area concern external aerodynamics, where turbulence has to be taken into account to model external complex flows around a complete geometry profile since the numerical simulations are still too costly to be a true part of the optimization process. SMASH is interested in defining suitable multigrid solvers for the Navier Stokes equations using unstructured finite volume discretization grids. In addition, the unsteady feature of turbulent flow problems encountered e.g. in vibration of some material structure and damaged material problems requires the need of LES type models (large Eddy Simulation techniques).

Space industry Another application area we are concerned with is the behaviour of space launcher engine using liquid fuel or powder propellents. Since the media involve very heterogeneous ingredients, two-phase modelizations as well as the study of free surface problems are needed

Automotive industry In Diesel engine, the new generation injection system technologies, use high pressure spray injection techniques. Our eulerian modelization techniques may be used to describe the first steps of atomization of the spray. These phenomena are preceded by a dynamic liquid-vapor transition phase during which the compressibility feature of the flow appears to be crucial.

4.3. Energy industry

The needs in numerical modelization are concerned with thermohydraulics for nuclear energy production centers (as CEA and EDF), flow problems in pipe lines for oil company industry (extraction, oil transport and refining) and all other industries related to energy production or chemical engineering.

In these industrial domains, turbines, boilers and pipes envolve very complex flows which often evolve either violently and/or at high speed, or on the contrary evolve very slowly with a large stabilization time. Describing those phenomena which are intrinsically two-phase type flow problems appears to be fundamental in studies of security issues against hazards (nuclear industry, oil-chemical industry or chemical engineering industry). The ability of a CFD code to treat efficiently and accurately the different phase flow regimes (gaz/liquid flows, bubbling flows, packet flows, liquid film and droplet flows etc.) is still problematic. In addition, when dealing with very low Mach number flows, the numerical complexity and difficulty are still increased.

4.4. Examples of other application issues

Multiphase modelization techniques may also find a place in other various application domains. That is for instance the case in astrophysics for modelling keplerian type flows in a proto-planetary system. This type of

study is currently done in the project in collaboration with astrophysicists to validate some scenarii of planet formation based on the accretion disk assumption.
Another interesting domain of application concerns multiphase flow problems in highly energy-giving granular media. Most of the existing CFD codes that aim to simulate those types of multiphase flows uses the Euler equation model closed by an equation of state defined for the fluid mixture. That necessarily assumes that the phase temperatures (or phase density ...) equilibrium holds without making sure that such assumptions remain pertinent to this type of flow problems. We can therefore enhance our efforts to define models in which the physics is better and widely described for such media.

5. New Results

5.1. Modelling

5.1.1. Mass transfer in two-phase flows

Participants: Olivier LeMetayer, Jacques Massoni, Richard Saurel.

This work [12] deals with the modelling of permeable fronts such as evaporation fronts that appear in cavitation systems. Such fronts are considered as discontinuities through which a non-equlibrium liquid transforms into a liquid-vapor mixture at thermodynamical equilibrium. In order to determine the kinetics of this transformation, the evaporation front is assumed to propagate at a maximal speed corresponding to the Chapman-Jouguet deflagation point. Using this particular kinetic relation, Rankine-Hugoniot relations are closed at such fronts and then it is possible to solve the associated Riemann problems. However, this kind of front is subsonic and conventional averaging scheme such as Godunov experiences difficulties in the numerical approximation of these flows. To overcome this difficulty, the reactive Riemann problem solution is embedded into the discrete equation method [1]. Numerical results validates this approach with comparison to experimental data. Some examples show that the same approach can be applied to the propagation of detonation fronts.

5.1.2. Detonation in heterogeneous energetic materials

Participants: Ashwin Chinnayya, Eric Daniel, Richard Saurel.

The computation of detonation waves in heterogeneous explosives involves compressible multiphase mixture due to the decomposition of the material. A new method [8] for the modelling of interface problems and multiphase mixtures has been developed in the particular limit where the phase pressure and velocities relax towards equilibrium. This method is a variant of the discrete equation method [1]. The new discrete model is adapted to reacting flows with mass, momentum and energy transfer. The model is based on pure material equation of state and no mixture equation of state is used. It is used here for the computation of the reaction zone of detonation waves. It is validated over a set of difficult test problems with known exact solution. Its multi-dimensional capabilities are shown over problems involving a large number of different materials.

5.1.3. Five Equation hyperbolic reduced model

Participants: Hervé Guillard, Angelo Murrone, Richard Saurel, Marc Grandotto [CEA, Cadarache].

This work [13] deals with the construction of a five equation two-phase flow model. Using asymptotic analysis, this model has been derived from a more general seven equation model proposed in [5]. This model is unconditionally hyperbolic and its mathematical structure is close to the structure of the single phase Euler equations. We have studied the behavior of this model in the low Mach number limit and obtained the limit equations for this model. A numerical approximation taking into account the characteristic of the singular low Mach number limit have been derived (see section 5.2.2). Results on this system have been presented at ICMF2004 [19].

5.1.4. Modelling of bubbly flows

Participants: Hervé Guillard, Roxanna Panescu.

The simulation of disperse bubbly flows is very often done with the use of the so-called "drift flux" model where the slip velocity between the dispersed and the continuous phases is specified by an algebraic relationship. This simple approach suffers from a severe drawback : Depending on the flow regime, the slip relationship can change and with it, the mathematical nature of the model that can switch from hyperbolic to a non-hyperbolic system. Using a Chapman-Enskog asymptotic analysis, we have derived a model for bubbly flow where the slip velocity is expressed by a Darcy type relation. This model is always hyperbolic with a clear mathematical structure. The present work aims to define a numerical approximation for this model.

5.1.5. Modelling of two-phase protoplanetary disks

Participants: Pierre Barge [Laboratoire d'Astrophysique de Marseille], Eric Daniel, Hervé Guillard, Satoshi Inaba [Dept of earth and Planetary sciences, Tokyo Institute of Technology].

A 2-D hydrodynamical code has been developed to study the interaction of gas and dust in protoplanetary disks [10]. Gas is considered as a compressible fluid while solid particules are treated as a pressureless gas. Due to the interaction between the two phases, solid particules lose angular momentum and energy and migrate toward the central star. This code has been used to study the so-called lifetime problem and has shown that taking into account the full coupling of the solid and gaseous phases, particules can survive 16 times longer than in the uncoupled case. This opens interesting perspectives in the continuous growth scenario for the formation of planetesimals. This code will be used for the study of other scenarii (for instance the vortex scenario of Barge and Sommeria).

5.1.6. Level Set formulation and Interfaces

Participants: Alain Dervieux, Anne-Cecile Lesage, Olivier Allain.

Works on level set formulation for the representation of interfaces have been done in collaboration with the Lemma company. Academical test cases on soliton propagation and bubble ascension [20] have been performed. Currently, the level set model is being improved by the use of Hamilton-Jacobi models to extend several key-variables fields, including those related to capillarity modelization.

5.1.7. Large Eddy Simulation (LES)

Participants: Simone Camarri [U. Pisa], Charbel Farhat [U Boulder], Alain Dervieux, Bruno Koobus [Montpellier2], Maria-Vittoria Salvetti [U. Pisa].

The purpose of this work is to devise new LES models suitable for industrial applications on unstructured meshes. Although, the characteristic Reynolds numbers of the considered problems are of the order of several millions, several zones of the flows can be more accurately computed with LES modelling than with usual statistical models. In particular, as shown in the popular Detached Eddy Simulations intiated by Spalart and his colleagues, the detached vortex zones can be treated by LES modelling. The approach followed in our group [17] is rather the one by Batten-Golberg-Chakravarthy, (LNS -Limited Numerical Scale). An article is submitted.

5.1.8. Acoustics in high speed flows

Participants: Ilya Abalakin [IMM-Moscow], Alain Dervieux, Tatiana Kozubskaya [IMM-Moscow].

Works on round-off errors in the NonLinear Disturbance Equation model have been published [6]. We now investigate viscous models. On the other hand, in the framework of a collaboration with Dassault-Aviation, a new 3-D superconvergent scheme has been devised. [24] This improvment has been used in the study of Large Eddy Simulation models (see section 5.1.7).

5.1.9. Statistical models and fluid-structure interactions

Participants: Charbel Farhat [U Boulder], Alain Dervieux, Bruno Koobus [Montpellier2], Eric Schall [University de Pau], Y Bentaleb [University de Pau], K El Omari [University de Pau].

Applications of statistical models of turbulence are done in collaboration with the University of Pau for the study of a giant and flexible Zeppelin-type airship. In these studies, the Reynolds number is extremely large. Currently, the numerical investigations concern low Mach number numerical methods, aeroelastic coupling and the treatment of turbulent boundary layers on anisotropic meshes. [16] [22] [21],[23].

5.2. Approximation

5.2.1. Pressure relaxation methods

Participants: Marie-Hélène Lallemand-Tenkès, Ashwin Chinnayya, Olivier Le Metayer, Richard Saurel.

Study of instantaneous pressure relaxation methods has been achieved this year and reported in a paper accepted in International Journal of Numerical Methods in Fluids [11]. Some generalization of these procedures in the context of multiphase flows with an arbitrary number of fluids have been studied.

5.2.2. Low Mach number flows

Participants: Hervé Guillard, Angelo Murrone.

We have extended the preconditioning techniques studied in [9] to more complex models than the single phase Euler equations and in particular to the five equation two-phase system derived in [13]. To deal with low speed flows, a preconditioned technique have been studied [25]. Numerical experiments have showed that these preconditioned techniques give excellent results and allow to compute flows close to the incompressible limit.

5.3. Parallelism and Grid Computing

5.3.1. Globus environment and Virtual Private Network

Participants: Jacques Massoni, Patrick Nivet, Hughes Digonnet [ENSMP].

The progress of the ACI-GRID2002 "MecaGRID" throughout this year can be summarized as follows : First, the establishment of a VPN (Virtual Private Network) based on protected tunnels has been finalized and tested. In a second step, the first tests validating the chosen solution (VPN + globus+ MPI) have been carried out with the clusters of the three sites using the application codes AERO3D and Stokes 3D. Those tests were conclusive. During this period, the CEMEF cluster has been updated and was removed from the grid. It needs now to be re-introduced in the grid.

5.3.2. Mesh partitioning for a computational grid

Participants: Hervé Guillard, Youssef Mesri, Hughes Digonnet [ENSMP].

The goal of this work done during the master thesis of Youssef Mesri was to improve the efficiency of a parallel mesh partition tool taking into account heterogeneous processors speed and communication time. In a previous work, we had devised a mesh partition algorithm that achieves load balancing with heterogeneous CPU while trying to minimize the communication time on an non-homogeneous network. However, this algorithm, was based on local operations. For very large meshes, this results in large CPU time to achieve the partition of a mesh. The new algorithm uses global operations to partition the mesh and reduces the CPU time in a significant manner.

5.3.3. Grid-enabled application codes

Participants: Alain Dervieux, Bruno Koobus, Steve Wornom.

In the context of the MecaGRID initiative, the Smash team develops a set of computational tools for demonstrations in Grid Computing. The central kernel is a CFD code (AERO) derived from the synthesis of research developed by the SMASH Team in collaboration with the University of Colorado at Boulder. This code executes in parallel using MPI and is natually suited for MPI Grid Computing. A new kernel, AEDIF derived from AERO, computes two-phase flows using a new diphasic models developed in the project ([13]). AEDIF solves the discrete equations on unstructured meshes using tetrahedras with an MPI parallel mode based on grid partitioning. Results obtained with this new kernel have been presented at [18]. This code has been ported on the MecaGRID and experiments with up to 64 processors localized on the three sites have been performed [26].

5.3.4. *Large Eddy Simulation on a computational Grid*

Participants: Alain Dervieux, Bruno Koobus, Vanessa Mariotti, Patrick Nivet.

Progresses made on the use of the computational grid MecaGRID allow to consider computations involving several millions of mesh points. In the framework of an internship, Vanessa Mariotti from the university of Pisa studies the turbulent interaction of a cross-jet with a pipe flow with LES/LNS turbulence models (see section 5.1.7).

5.3.5. *Parallel code for interface simulation*

Participants: Youness Bouraze, Jacques Massoni.

During the internship of Youness Bouraze, a parallel Fortran 90/MPI based code has been written for the simulation of compressible multi-fluid flows. The parallel strategy is based on domain decomposition. This code has been tested on unsteady problems involving more than 2 millions of unknowns with a relative speedup on 28 processors of the order of 15.

5.3.6. *Distributed Mesh applications*

Participants: Mohamed Essaidi, Patrick Nivet, Hervé Guillard.

For current applications of metacomputing in CFD, the meshes can involve millions of points and elements and cannot anymore be stored in the memory of a single processor. In this framework, all the basic I/O operations, creation of data structures (e.g creation of the CSR format to store the mass and stiffness matrices) or geometrical operations associated to unstructured Finite Elements or Finite Volume methods have to be performed from the begining in a distributed context. This is the starting point of this new study whose aim is to create an OO library for the handling of very large Finite Element unstructured meshes in a distributed environment.

6. Contracts and Grants with Industry

6.1. Modelling of bubbly flows

Participants: Hervé Guillard, Roxanna Panescu.

In the framework of a preliminary program to study convective pattern in bubbly flows, IRSN and Smash have engaged an initiative for the numerical modelling of bubbly flows.

6.2. Level-Set software

Participants: Alain Dervieux, Anne-Cécile Lesage.

The subject of this partnership with the technological company LEMMA is to develop a level-set based multi-fluid software for applications in the aerospace industry.

7. Other Grants and Activities

7.1. National and Regional initiatives

7.1.1. *Ministry Grant ACI-GRID "MECAGRID"*

Participants: Olivier Basset, Thierry Coupez [Ecole des mines de Paris], Hughes Digonnet [Ecole des mines de Paris], Hervé Guillard, Jacques Massoni, Patrick Nivet, Richard Saurel.

This initiative launched in November 2002 associates the CEMEF of Ecole de Mines de Paris, IUSTI of the University of Provence and INRIA in the construction of a computational grid from three PC clusters located in the PACA region. This grid will be devoted to massively parallel applications in multimaterial fluid mechanics.

7.1.2. Collaboration with University of Pisa

Participants: Maria-Vittoria Salvetti [University of Pisa], Francois Beux [University of Pisa], Vanessa Mariotti [University of Pisa], Simone Camarri [University of Pisa], Hervé Guillard, Alain Dervieux.

Through its support program for the development of regional research centers, the Conseil regional de la région PACA supports a collaboration with the University of Pisa on the development of numerical models for two-phase flows.

8. Dissemination

8.1. Teaching

Project members have teached the following courses :

Mécanique des fluides compressibles : cours de Maîtrise d'Ingénieurie Mathématique, University de Nice-Sophia Antipolis, 20 h (H. Guillard).

8.2. Ph. D thesis and Masters Thesis

This year, the project has harboured the following Ph. D Students :

ROXANNA PANESCU University of Nice-Sophia-Antipolis, "Méthodes de volumes-Eléments finis pour les écoulements de liquides à bulles"

ANNE-CÉCILE LESAGE University of Nice-Sophia-Antipolis, "Méhodes numériques pour les écoulements diphasiques"

OLIVIER BASSET ENSMP, "Simulation numérique de mousses sur grille de calcul"

The following masters thesis have taken place :

YOUSSEF MESRI "Partitionnement de maillage sur une grille de calcul", DESA de Mathématiques Appliquées, University of Meknes, Morroco.

YOUNESS BOURAZE "Simulation numérique d'écoulement à interfaces", ISIMA (Institut Supérieur d'Informatique, de Modélisation et de leurs Applications, Clermont-Ferrand).

8.3. Conferences and Seminar Organization

- In june 21-25 2004, the project has organized the international conference "Mathematical and Numerical aspects of Low Mach number flows" that has gathered around sixty mathematicians and numeriscist working on this topic (see http://www-sop.inria.fr/smash/LOMA/main.html).
- Richard Saurel and Hervé Guillard are members of the scientific committee of CFM2005 (Congrès Français de Mécanique).

8.4. Conferences and workshops

Project members have participated to the following conferences and seminars:

- A.Dervieux, Invited conference at 16eme Seminaire CEA-GAMNI de Mecanique des Fluides
- A.-C. Lesage has presented a paper in "Mathematical and Numerical aspects of Low Mach Number Flows", June 21-25, Porquerolles, France.

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Major publications by the team in recent years

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