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Numerické metody pro lagrangeovské a lagrangeovsko-eulerovské hydrodynamické simulace

Numerical Methods for Lagrangian and ALE Hydrodynamic Simulations

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Summary

This presentation summarizes some outputs of research and other contributions in the field of numerical methods for Lagrangian and Arbitrary Lagrangian-Eulerian (ALE) hydrodynamic simulations of laser-plasma interaction, on which its author collaborated in recent years. Particular topics include new types of artificial viscosity, consistent treatment of the equation of state, strategies for symmetry preservation at various stages of the ALE algorithm, techniques for effective and solution-aware mesh rezoning, methods for synchronized flux-corrected remapping (FCR), and some examples of real applications. Directions of ongoing research and plans for near future are mentioned.

Keywords:Arbitrary Lagrangian-Eulerian methods,
Artificial viscosity,
Equation of state,
Rezoning,
Remapping,
Symmetry preservation,
Hydrodynamic simulations

Souhrn

Tato prezentace shrnuje některé výsledky výzkumu a další příspěvky v oblasti numerických metod určených pro lagrangeovské a lagrangeovskoeulerovské (ALE) hydrodynamické simulace interakcí laseru s plazmatem, na kterých měl jeho autor tu čest v poslední době spolupracovat. Mezi pojednávanými tématy jsou nové typy umělé vazkosti, konzistentní vyhodnocování stavové rovnice, strategie zachování symetrie v různých fázích algoritmu ALE, účinné a k řešení citlivé techniky adaptace výpočetní sítě, metody typu FCR (Flux-Corrected Remap) pro konzervativní přenos řešení mezi sítěmi a příklady konkrétních aplikací z praxe. Dále jsou zmíněna témata autorova současného výzkumu a naznačeny plány do budoucna.

Klíčová slova:	Lagrangeovsko-eulerovské metody,
	umělá vazkost,
	stavová rovnice,
	adaptace sítí,
	remap řešení,
	zachování symetrie,
	hydrodynamické simulace

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1 Introduction

The task of computational fluid dynamics is to grasp fluid dynamics using numerical methods and algorithms. Usually, partial differential equations are discretized and the set of resulting algebraic equations is solved using a computer. This presentation is pointing up some modest contributions to this vast area of research. Suggested methods are exposed here in the framework of hydrodynamics described by Euler equations with some added mechanisms allowing to simulate the interactions of laser radiation with plasma and solid targets under warm dense matter conditions, however most of the presented techniques can be directly used or easily modified to work under other circumstances, too.

There exist several ways to approach the hydrodynamic calculations on computational meshes. For example, the problem can be described either using the Lagrangian or the Eulerian formalism, the equations can be discretized on the computational mesh either in the cell-centered or the staggered manner, etc. Most of these basic paths have been followed for decades, and many achievements of particular methods can be found in the literature, where their advantages are leveraged and their drawbacks fought. It seems reasonable to build on this knowledge and, rather than condemning some methods and advocating for others, try to advance and/or combine them to suit to the simulation of a given type of physical problems. A very successful combination of the Lagrangian and Eulerian description and their related techniques is the Arbitrary Lagrangian-Eulerian (ALE) methodology.

This text is presenting some recent new contributions and modifications to the methods employed in the ALE framework, focusing on aspects such as the thermodynamic consistency of the equation of state (EoS), artificial viscosity, the preservation of symmetry by the Lagrangian scheme and elsewhere, or conservative remapping of the state variables between computational meshes. The aim of this presentation is not to give a full summary and description of the current methodology, but to briefly recall some particular aspects of ALE simulations and related methods on which the author recently had the honor to collaborate and put the results of this work into the context of current research in the computational fluid dynamics community.

The rest of this document is organized as follows. Section 2 introduces the basic terminology and popular approaches in ALE framework. Section 3 then highlights some aspects of the calculations and related particular techniques. Finally, some of the current research, activities and plans of the author are outlined in Section 4. References to the papers featured in the habilitation thesis [84] will be [highlighted] to be distinguished from standard [references] to other works.

2 Arbitrary Lagrangian-Eulerian (ALE) Calculations

Historically, there have been two basic ways to observe and describe the flow of the fluid: the Lagrangian formulation and the Eulerian formulation. The Lagrangian observer follows a specific fluid parcel, as it moves and evolves in time and space, while the Eulerian observer is detailing a specific spatial region, with the fluid coming and going. Typically, deciding between these two frames of reference has been compared to either throwing objects into the river and following them, or sitting at the river and observing the floating objects passing by. Applied to fluid dynamics calculations on computational meshes, each of these approaches has its advantages and drawbacks. The tempting property of the Lagrangian description is that the advective terms of the fluid equations vanish thus, for example, each element (cell, subcell, etc.) retains its constant mass throughout the calculation. The Lagrangian meshes are moving with the fluid, which is useful to represent processes with swift size and shape changes of the computational domain due to rapid compression and expansion, and also allows to some extent to naturally follow features in the solution such as shock waves, contact discontinuities or material interfaces. At some point, however, the moving mesh can become too deformed, which may lead to a catastrophic loss of accuracy, or even a deadlock and failure of the calculation. This should not happen in Eulerian calculations, where the mesh does not move in time, and from this viewpoint the Eulerian calculations are more robust, however here the challenge is to maintain sharp features and interfaces in the solution by keeping the inherent diffusiveness of this approach in control. A lot has been written on pros and cons of the Eulerian and Lagrangian approaches. For more insight and examples, see e.g. [21, 66, 13].

The main idea behind the Arbitrary Lagrangian-Eulerian methods is that these two approaches described above can be considered as being extreme cases of a *general* mesh motion. That is, when the mesh elements are not moving at all, the calculation is Eulerian, while when they are moving entirely with the fluid, as if each mesh node was connected to some fluid particle, the purely Lagrangian description is recovered. In ALE calculations, the motion of the mesh is not limited to these two ex-



Figure 1: Simulation of a point-symmetric shock wave (centered at the lower left corner of the plots) on an initially regular honeycomb mesh. Left: pure Eulerian calculation; right: pure Lagrangian calculation; center: Arbitrary Lagrangian-Eulerian (ALE) calculation

tremes. The middle panel of Fig. 1 shows the point-symmetric explosion as simulated by the ALE method, while pure Eulerian and pure Lagrangian results are seen on the left and right side, respectively. The origins of the idea to combine the Lagrangian and Eulerian approach and thus benefit from this synergy are hard (if not impossible) to track, but it is often attributed to the seminal work of W.F. Noh in the 1960's. In 1974, the important paper by Hirt et al. [39] summarized the state of the art of the Lagrangian-Eulerian techniques and suggested to formulate the Arbitrary Lagrangian-Eulerian (ALE) method as a procedure consisting of three repeating blocks: (I) the Lagrangian phase, where the mesh moves along with the fluid with no advective intercell fluxes, (II) mesh rezoning, where the mesh is improved by sensitive smoothing or topology changes in order to prevent distortions and maintain the accuracy, and (III) mesh remap*ping*, where the solution is transferred from the old (Lagrangian) mesh to the new (rezoned) one in a conservative manner and with sufficient accuracy. The evolution of the mesh and the solution (state variables) at these



Figure 2: Stages of the indirect ALE algorithm. Clockwise from top left: Lagrange step (advance in time), rezoning (mesh adaptation), remapping (transfer of solution onto the rezoned mesh)

stages is demonstrated in Fig. 2. In this text we adopt this three-step formulation, sometimes referred to as *indirect ALE* method, however let us remark, that another valid and popular way to combine the Lagrangian and Eulerian approaches is the *direct ALE* method [24, 34], where advection is directly embedded in the equations, so that the mesh is being adapted continuously during the calculation. Worth mentioning is also the Lagrange Plus Remap method [70, 93], where the rezoning step consists in simply returning the mesh back to its original state after each Lagrangian step. Over the years, reported advances in the field of ALE calculations have been occasionally condensed in review papers such as [39, 6, 68, 4].

To represent the state variables on the computational mesh, one can use the *staggered* discretization, where the values of thermodynamic variables (such as density or pressure) are assigned to cells and the kinematic variables (position, velocity) to mesh nodes, or the *cell-centered* discretization with all variables primarily assigned to cells. In other words, while in the cell-centered approach the control volumes are cells, in the staggered schemes the control volumes for integration are alternating between primary (real) and dual (node-assigned) cells.

The origins of staggered methods can be traced back to the seminal works of von Neumann and Richtmyer [95]. While mass conservation is ensured by declaring the cells Lagrangian objects and momentum conservation is typically achieved by discretizing the momentum equation in a conservative form (using numerical fluxes), the conservation of total energy remains to be guaranteed by the construction of the particular scheme. Great advances in this sense have been achieved using mimetic methods [74, 80], ensuring that the discrete operators are analogs of their continuous counterparts, and compatible discretizations using the concept of subcells and dual grids [12, 13]. Since the staggered discretization of equations corresponds to inviscid flow, one of the biggest challenges here is the proper treatment of entropy due to the dissipation of energy across shock waves in the fluid. This is the main purpose of artificial viscosity, which will be discussed in Section 3.1.

In the cell-centered discretization, the mesh cell can be viewed as a control volume moving with the fluid, and thus cell-centered hydrodynamics is also referred to in the literature as Finite Volume method on moving grids. Unlike the staggered approach, here the total energy is conserved automatically, because its equation is being solved directly in its conservative form. On the other hand, since velocity is now primarily assigned to cells, the velocity of nodes must be approximated by the scheme in a compatible manner so, that the resulting mesh motion satisfies the socalled *Geometric Conservation Law* (GCL), which can be viewed as the requirement that the temporal change of cell volume due to mesh motion (calculated from the mesh geometry) is the same as the volume change obtained by the solution of the discrete conservation equation, see e.g. [66] for details. Because the velocity used to move the mesh is calculated by solving Riemann problems, as it was done in its simplest form in the iconic Godunov scheme [35], the cell-centered techniques are also frequently referred to as Godunov methods in literature. As in the case of staggered discretization, also the cell-centered methods have gradually evolved into robust and accurate tools for practical calculations, see [84] for a list of some milestones.

The mathematical formulations above are clearly not the only ones in which the ALE methods for hydrodynamics are being developed. Impressive results have been achieved for example using the Finite Element description [23] and other variational methods, which are however beyond the scope of this presentation, as are many sophisticated techniques using curvilinear meshes, high-order reconstruction of functions, multimaterial cells, mesh reconnection, etc. Besides the already mentioned overview in [4], a rich source of information about these ideas and their applications are the regular MULTIMAT conferences on numerical methods for multimaterial flows [1].

3 Selected Aspects of the ALE Methodology

Now let us focus on selected parts of the ALE machinery and some aspects of the ALE simulations. Rather than to proceed blockwise, that is, start with the Lagrangian phase and then advance to the rezone and remap stages, this presentation is organized by topics, some of which relate to more than one step of the ALE algorithm. While the artificial viscosity (Section 3.1) is typically employed in the Lagrangian step of staggered methods to prevent the collapse of the mesh due to passing shock waves, we will show that some of its forms can also be seen as a bridge between staggered and cell-centered schemes. To preserve symmetry for symmetric problems on conforming meshes (Section 3.2), caution has to be exercised in the Lagrangian step, when rezoning as well as while remapping. Similarly, the equation of state (Section 3.3) is closing the system and thus it can be needed throughout the calculation, with its proper evaluation being crucial to get realistic simulation results. New techniques for rezoning and remapping are put into the perspective of recent advances and current trends in Sections 3.4 and 3.5. Finally, Section 3.6 offers a small sample of real applications in which the ALE simulations have been used and where even small modifications of employed methods yielded a substantial improvement of the results.

3.1 Artificial Viscosity

Due to the nature of staggered grid methods, namely due to the fact that this discretization corresponds to the inviscid flow, special care has to be taken to ensure the satisfaction of the second law of thermodynamics. In other words, a mechanism has to be employed that dissipates the energy (converts kinetic energy into internal) across the shock wave. This has been recognized in the very beginning and already von Neumann and Richtmyer [95] suggested to use the concept of *artificial viscosity* for this purpose. While in one dimension this is relatively simple, it turned out



Figure 3: Even small modifications to simple types of artificial viscosity such as CSW [14] or CS [11] can significantly improve the results [92]

that in multiple dimensions it is a challenging task to formulate an artificial viscosity that ensures dissipation, prevents the computational mesh from collapsing due to the passing shock waves, resists nonphysical mesh deformation and at the same time respects the direction of flow. In practice, a proper implementation is of highest importance for the stability and accuracy of calculations with staggered schemes.

Probably the simplest approach in multiple dimensions is the so-called bulk viscosity, which amounts to adding an extra scalar term with the dimension of pressure into the cells being compressed, in order to prevent their collapse [95, 97]. This is however not sensitive enough to the solution (directions of flow) and cannot resist some harmful modes of mesh deformation [14, 49]. The idea of so-called edge viscosity, pioneered in [77] and developed e.g. in [14], is to employ and control the artificial viscosity along the mesh edges, depending on the expansion or compression of their attached subregions. This approach turned out to be very effective and is in fact frequently used in real simulation codes, especially because it does not overly damp physical vorticity. Some of its weaknesses, such as significant mesh imprint in certain situations [11], can be mitigated and the method made viable often by a few very simple modifications as we have shown in the short note [92]. Comparing the middle and left panel in Fig. 3, we see how the mesh imprint was reduced and symmetry improved by a mere change of a switch in edge viscosity. Addition of a simple term for the exchange of internal energy between cells acts similarly and moreover prevents the ubiquitous wall heating effect (Fig. 4, compare also lower vs. upper row in Fig. 3). However, the results are still



Figure 4: Wall heating can be avoided or reduced by addition of a simple energy exchange term [92]

not perfect in all calculations and thus the quest for a better and generally applicable artificial viscosity continues. There is a general agreement, that employing tensors should help to better follow features in the solution, for example by capturing the direction of shock propagation, and at the same time stabilize the mesh motion [76, 97]. Several so-called tensor viscosities have been suggested, be it the classical approach by Campbell and Shashkov [11] (CS), its generalization for arbitrary mesh topologies [53], or techniques to be used in the context of cell-centered schemes [3] or finite elements [49]. Very recently, a new wave of papers on this topic has been published.

As it has been mentioned above, while it is absolutely necessary in staggered schemes to provide artificial viscosity or some similar mechanism with the same effect, it is not the case in cell-centered schemes based on Godunov's method [35], where the dissipation of kinetic energy into internal energy is inherently provided by the solution of the Riemann problem, see [19, 25] for details. In a recent series of papers we have developed the idea to use the same mechanism in the framework of staggered schemes. The solution of a Riemann problem located at the cell center provides the cell-centered velocity, which is then used in the viscous force assigned to the particular subcell. The motivation for this approach was the following consideration: If the staggered and cell-centered approaches are two paths to the same objective, then artificial viscosity should emerge from the difference between them, and at the same time serve as the bridge between the cell-centered and staggered machineries. This concept, which



Figure 5: Simulation of a hydrodynamic instability using classical edge artificial viscosity (left) and the new method [61] based on cell-centered Riemann solver (right)

was demonstrated in two [60], [67] as well as three dimensions [61], see also Fig. 5, seems to have (re)gained attention and further resonates in recently published works.

Another important topic is the application of artificial viscosity in cylindrical (axi-symmetric, r-z) coordinates. The popular approach of area weighting (AW) allows the schemes designed for planar geometry to be easily applied in r-z, basically by just multiplying the nodal force by the *r*-component of the node's position. While this preserves spherical symmetry for symmetric problems on conforming meshes, unfortunately some other properties of the schemes can be lost. For example, the areaweighted CS tensor viscosity [11] is not strictly dissipative anymore, which violates the second law of thermodynamics. In [90], [89], we have proposed a method that is genuinely r-z, dissipative, conserves the z-component of momentum, preserves spherical symmetry on equi-angular polar grids, and can be applied on any mesh topology with no need to tinker around with problem- or mesh-dependent parameters. Its typical outcome on polar grids in Cartesian geometry and on logically rectangular grids in cylindrical (r-z) geometry, as compared with the benchmark AW CS tensor viscosity, is shown in Fig. 6.

Since a robust and universal artificial viscosity is in high demand but still elusive, many interesting improvements are being published persistently. For example, the concept of hyperviscosity is trying to overcome the fact that the classical artificial viscosity is only first-order accurate by using it in a way that allows higher order of accuracy on regions with



Figure 6: Comparison of area-weighted Campbell-Shashkov tensor artificial viscosity [11] (upper row) to the new genuinely r-z approach LapEdge [90] (lower row)

smooth flow. Recently, hyperviscosity was applied to finite element ALE calculations with impressive results [5].

3.2 Preservation of Symmetry

Among the physical problems studied with the help of ALE simulations are very often those with spherical or cylindrical symmetry, which can be encountered in various application areas such as laboratory astrophysics or inertial confinement fusion. Due to the extreme conditions, any deviation from perfect symmetry may trigger hydrodynamic instabilities, such as Kelvin-Helmholtz, Rayleigh-Taylor or Richtmyer-Meshkov [27]. In these simulations it is very important that the numerical scheme preserves the symmetry, if it exists in the physical problem under study. That is, numerical error must not render the (theoretically symmetric) solution non-symmetric or unstable. Moreover, for technical reasons, sometimes the calculations are preformed in different coordinate systems, for example one might want to calculate some three-dimensional problem with spherical symmetry using a two-dimensional cylindrical (r-z) calculation. A properly chosen scheme should not break symmetry in this case but rather stabilize the simulation. As observed and demonstrated by Benson [6], symmetry is highly desirable primarily for geometrical robustness.

Of course, in the indirect ALE algorithm, all its stages have to preserve symmetry. It would make no sense if a perfectly symmetric Lagrangian solution was remapped to a rezoned mesh in a non-symmetric manner.

In the field of cell-centered Lagrangian schemes, Maire was well aware of the importance of symmetry preservation and the fact that the control volume scheme as such is lacking this property, and thus immediately extended his well-known Cartesian scheme [65] to cylindrical coordinates [64] using the area-weighted approach (which was already mentioned earlier in Section 3.1 in the context of artificial viscosity), presenting a scheme that preserves radial symmetry on equi-angular polar grids. However, the principal drawback of the AW technique is the fact that the actual integration is performed over planar areas instead of over real volumes, making the resulting methods prone to difficulties such as violating the conservation of momentum and energy, which must then be ensured explicitly, often with complicated or expensive corrections. Therefore, in [16, 17, 18, 52], Cheng, Shu and Ling presented an impressive amount of work done to develop cell-centered Lagrangian schemes that maintain symmetry and possess other beneficial properties, such as positivity preservation (avoiding nonphysical negative values of internal energy due to small differences of large similar numbers) and, of course, GCL conservation.

As for the staggered schemes, symmetry preservation was studied for example in [15], where it was shown that on quadrilateral cells in r-z, preservation of spherical symmetry, perfect satisfaction of the GCL, and total energy conservation are incompatible even on conforming grids. There are schemes which do not preserve symmetry in r-z at all, and others that can be used in r-z by area weighting of a Cartesian method, and thus preserve symmetry, but do not satisfy the GCL - examples of both can be found in [12]. In [62], GCL is restored by time integration using Simpson's formula instead of trapezoidal rule, but again at the price of symmetry violation. We have further explored this idea and in [91] suggested a method that preserves symmetry and conserves total energy by construction, while reducing the GCL violation to the order of entropy error. In particular, the forces from the volume consistent scheme [62] are corrected so, that spherical symmetry is preserved on an equi-angular polar mesh. Fig. 7 shows how this new method compares to its predecessor [62] and to a typical Cartesian scheme applied in r-z using the area-weighted approach. Moreover, we suggest in this paper how to symmetrize other schemes by this technique, and demonstrate this idea on the method referred to as control volume scheme in [12].

It was already discussed above, that staggered schemes must also be supplied with a suitable artificial viscosity for stabilization and prevention of mesh collapse due to passing shock waves. Clearly, this must not destroy symmetry either. Again, a suitable Cartesian approach can be applied in r-z using area weighting, but this may have side effects such as the loss of



Figure 7: Coggeshall test (adiabatic compression) calculated by an area-weighted scheme, the volume consistent but non-symmetric GC scheme [62], and the symmetrized scheme GCS [91]. Top: computational mesh, bottom: evolution of logarithm of L_1 error in time

strict dissipativity, which is a serious flaw of any artificial viscosity, since it violates the second law of thermodynamics. To avoid this, we have constructed a genuinely r-z artificial viscosity [90],[89], already mentioned in Section 3.1, which is strictly dissipative while preserving spherical symmetry on equi-angular polar grids and yields reasonable results also on other structured quadrilateral meshes (confront Fig. 6 again).

Furthermore, on the way toward symmetry improvement in the Lagrangian step, our schemes [60], [67, 61] carry out the limiting of interpolation slopes in directions given by the local flow, rather than in coordinate directions.

Finally, for an example of a method constructed to preserve symmetry in the remap phase, the reader is referred to [94], where we are transforming and remapping the velocity vectors along the directions aligned with local flow, respecting coordinate invariant local bounds, which greatly improves the radial symmetry of remapping on conforming meshes. This will be also discussed later.



Figure 8: Inconsistent evaluation of EoS can provide nonsensical results such as negative density or pressure (top left), spurious oscillations in dependency of state variables (top right), or thermodynamic potentials not being potential functions (discrepancy at bottom left). The HerEOS tool [101] can provide reasonable results even from imperfect EoS data by thermodynamically consistent interpolations (bottom center) and replacement of data for problematic variables by finite differencing (bottom right)

3.3 Equation of State

To achieve realistic results in hydrodynamic simulations of laser-plasma interactions, it is crucial to employ a correct hydrodynamic closure and properly evaluate the equation of state (EoS). A good EoS correctly describes the state of a material (or mixture) under given physical conditions by relating the thermodynamic state variables such as pressure, temperature and internal energy. Depending on the particular range of parameters (e.g. temperature, density or laser intensity), one has to choose a suitable EoS model or combination of models to stay physically relevant and in good correspondence with experimental data. Currently, there exist many EoS models and libraries, which vary not only in their primary purpose, complexity and availability to the general public, but also in the extent to which they are balancing computational efficiency, robustness and the level of satisfaction of fundamental thermodynamic relations. Technically, two types of EoS can be encountered. In the simpler (*inline*) case, represented for example by the Quotidian equation of state (QEOS) [69], the values of state variables such as pressure or entropy can be directly calculated at any point of the (say) density-temperature space, using relations based on some theoretical or semi-empirical model. Unfortunately, this is typically fairly expensive due to the necessity to solve nonlinear problems. EoS of the other type, such as the Los Alamos library SESAME [63], are based mainly on measured experimental data and provided only as tables of discrete values of selected state variables, with spacing far from ideal.

It is rather surprising that there exist established hydrodynamic simulation codes using very sophisticated and accurate numerical methods but paying not enough attention to the choice and consistent evaluation of the EoS closure. In particular, it is not uncommon to encounter EoS libraries providing negative values of density or pressure in some regions (sometimes with inconsistent *a posteriori* corrections), oscillating dependencies of variables on each other, or thermodynamic potentials not being potential functions - see Fig. 8 for some examples. Our HerEOS library [101] seeks to remedy this situation by suggesting a tool for the evaluation of an arbitrary EoS (selected or provided by the user) in a fast, robust and thermodynamically consistent manner, using higher-order interpolations of some thermodynamic variable, such as Helmholtz free energy. This ensures that the returned values of derived variables are respecting correct dependencies, so that the data provided by HerEOS are physically meaningful and thermodynamically consistent, as long as the employed EoS itself (inline or tabulated) is reasonably consistent. We have tested and practically used the HerEOS tool in several simulation codes with various EoS, such as QEOS [69], FEOS [28], BADGER [38] and SESAME [63].

3.4 Rezoning

From the logic of the ALE method it is clear, that the rezoning step should not contradict the Lagrangian spirit of the previous calculation, so that as much precious information as possible (e.g., sharp shock fronts and interfaces) is carried along after the remapping. On the other hand, at some level of mesh deformation the truncation error due to finite differencing with irregular spacing would start to prevail over the numerical diffusion due to remapping. Moreover, extremely deformed elements may dictate a very short time step, so that it would be too time-consuming or even impossible to arrive at the intended final time of the calculation. Therefore, preserving proper mesh quality is crucial to prevent premature failure of the calculation and maintain sufficient accuracy.

For the numerical scheme to stay relevant, the mesh must definitely be valid, that is, not tangled. In a mesh of triangles, tangling can only happen when some cells become flipped, so that their volume is negative in the sense of the original orientation. For general polygonal cells, tangling occurs also when they are only partly inverted. A typical example is the hourglass, or bowtie (\bowtie) , deformation of quadrilaterals, where only a part of the cell volume becomes negative [13]. A description of a few more notoriously harmful deformation modes on polygonal meshes in 2D can be found in [78, 83], along with a suggestion how to treat them. And a real zoo of mesh deformation types exists and has to be dealt with in three dimensions. A mesh that is valid (by prevention or after untangling) must still be improved in quality. What exactly that means depends on the application, particular problem, and the user's taste. For example, some Lagrangian schemes require all mesh cells to be not only valid, but also convex. There exist also rezoning approaches that can be primarily used to maintain reasonable mesh quality throughout the ALE calculation, but are able untangle it if something goes wrong [86, 7].

There are several strategies used to adapt the mesh, such as local mesh refinement (also referred to as h-adaptation), node reconnection (*c*-adaptation), or mere movement of mesh nodes without changing the connectivity (*r*-adaptation). While the latter is seemingly the most natural for the Lagrangian description of smooth flow and the simplest for bookkeeping, phenomena such as shock waves or dramatic shear flows can render it insufficient at some point, and require connectivity changes or complete remeshing.

Some of the oldest pure geometrical methods for mesh generation and relaxation were proposed by Winslow [98, 99], Brackbill and Saltzman [10] and later analyzed and extended in many works, e.g. by Knupp [44, 45] and others. To achieve a good mesh quality while preventing oversmoothing, various criteria are often taken into account and combined, such as smoothness, cell size and orthogonality, both on the global and the local scale. One of the simplest indicators of local mesh quality is the *condition number* of the Jacobian matrix, a fundamental theoretical object in mesh generation, representing the map between the unit (canonical) simplex and the mesh element corner [43, 44, 46, 47]. Several successful methods are fully or partly based on the optimization of the condition number, or can be interpreted by its means, be it the elaborate Reference Jacobian method [48, 26] or the efficient rezoning strategies for 2D and 3D curvilinear meshes using high-order parametric mapping and yielding impressive results [2, 4].

As said above, especially in indirect ALE calculations the mesh de-



Figure 9: Adaptation of various meshes to an underlying function by weighted condition number smoothing [88]

formation reflects the fluid flow under study. Therefore a good rezoning strategy should consider not only the mesh geometry, but also the physics of the problem, for example by estimating the discretization error of some representative state variable in the actual solution, accounting for its gradients, or employing fluid velocity in the mesh quality indicator. This may produce meshes which are not smooth visually, but have the cells aligned so, that the numerical error remains reasonable also in highly anisotropic regions and across steep gradients. We suggested a method [88] where the mesh is rezoned by the optimization of a condition number based objective function complemented by an arbitrary weight function. The weight can be either given by some smooth function with values and derivatives known everywhere, so that the mesh is adapted according to some coordinate system or focuses on some specific regions of interest, or it can be given by discrete values assigned to the mesh elements, for example of actual density or of any other state variable, so that the mesh aligns with the solution. Examples of adaptation of three different kinds of mesh to two different underlying functions can be seen in Fig. 9. This technique was further extended, applied in Lagrangian simulations and, using a barrier function as a weight, for dynamic tracking of material interfaces [36]. Recently, discrete simulation fields have been also employed for the adaptation of curvilinear meshes in ALE calculations [22].

Besides pure node movement methods, there exist many rezoning strategies involving adaptive mesh refinement and derefinement, node reconnection, etc. In [85], we used the so-called *edge swapping* technique to rezone an unstructured triangular mesh so, that the discretization error of some prescribed function or state variable is minimized. Very interesting and inspiring is also the employment of Voronoi tessellations, where the adaptation of mesh or its part consists in constructing it anew from updated generators, so that the connectivity may change, but the new mesh is in a sense close to the original one and moreover retains some nice properties, such as the cell faces given by any number of vertices staying planar in three dimensions. An early example is the so-called ReALE method [59], for a more recent utilization see e.g. [34]. However, even a brief overview of existing solution-sensitive adaptation strategies for various kinds of computational meshes is far beyond the scope of this text.

3.5 Remapping

In the indirect ALE algorithm, the remapping step serves to interpolate the state variables from one mesh, resulting from the Lagrangian phase of the calculation, to another mesh, which is improved so that the calculation can continue flawlessly.

Transferring the solution between two general computational meshes requires their overlay and calculation of intersections. However, in the very common case when the new mesh has the same connectivity as the old one (that is, rezoning was carried out only by moving the nodes, not by reconnecting them or by complete remeshing) and the cells of the new mesh are not far away from their counterparts in the original mesh, it is useful to formulate remapping in terms of intercell fluxes.¹ To maintain sufficient accuracy, high-order interpolation is preferable, which however tends to produce local extrema, that is, overshoots and undershoots with respect to values in neighboring cells (violation of local bounds). One option to deal with this is the *a posteriori* repair [79], which simply redistributes these bumps or dips into the surroundings, regardless the flow direction. An alternative approach is trying to a priori prevent the spurious oscillations due to the unlimited high-order fluxes, rather than mitigating the damage already done. It is based on the Flux-Corrected Transport (FCT) technique [9, 100, 75, 50], where a failsafe (always boundpreserving) low-order flux is combined with a high-order flux so that as much of the latter as possible is used but the local bounds are still preserved, that is, the maximal and minimal values of selected variables in

¹At this point let us remark, that while this is sometimes called (mesh) advection, it is not advection in the sense of physics: no physical quantities are evolved in time at the rezone and remap stages of the ALE algorithm. However, due to the the analogies of remapping with real advection, the term flux (in pseudo-time between cells of the two meshes) and the advection equation are sometimes used here.



Figure 10: The principle of flux-corrected remapping (FCR): use as much of high-order fluxes as possible while preventing overshoots and undershoots (preserving local bounds) by falling back toward low-order fluxes where necessary [56]

the local neighborhood of the actual cell are not exceeded. While FCT was originally designed for the simpler case of transport equations, FCR stands for Flux-Corrected Remapping and refers to the application of this idea to conservative remapping in hydrodynamics in general.

The focal point of the FCR approach is the set of so-called *correction* factors (to be denoted C here), which control the amount of antidiffusive fluxes to be used, that is, how close to the unlimited high-order method the intercell fluxes can be pushed while still preserving local bounds in cells. (The typical behavior of a low-order, high-order and FCR method on a shock wave is demonstrated in Fig. 10.) This is not a trivial task, since the system under study consists of coupled equations, and the constraints may be applied to other quantities than the conserved ones, to which the fluxes correspond. The particular FCR methods vary in the ways how the equations are processed (sequentially or simultaneously), which constraints are taken into account, and how the space of correction factors is searched for an optimum. Our older simple approach [87] employs the equations sequentially, that is, first finding C's for mass, then adding momentum, and finally the energy. Because the factors C for each newly added equation are multiplying the C's from the previously evaluated equations, and because the value C = 0 corresponds to the safe low-order method, the added corrections cannot break the already processed bounds. However, this may lead to overcorrection, where for example a jump in velocity or energy can overrestrict density, pushing it towards low order even when it is smooth and thus its high-order fluxes would also preserve the bounds. Therefore, with the SFCR (Synchronized Flux-Corrected Remapping) method [55], we are searching for the



Figure 11: Velocity magnitude for a point-symmetric problem with cyclic remapping on a logically rectangular mesh. Low-order remap (top left), unlimited high-order remap (top right), component-wise FCR in coordinate directions (bottom left) and symmetric FCR (bottom right) [94]

best correction factors for mass and momentum at the same time, imposing bounds on density and velocity at once. The polygonal phase space of admissible correction factors for mass and momentum is easy to search. In [56] we took another step by adding the fluxes of total energy and constraints on internal energy to the mix. As this introduces nonlinearity and thus renders the optimization-based search for ideal C's expensive, a simple trick is suggested, which first tries the admissibility of C's at their maximum (corresponding to pure high-order fluxes), thus effectively avoiding the actual optimization in smooth regions and only performing it in a few troubled cells, typically near the shocks or steep gradients. An important aspect of FCR is the symmetry preservation, which we investigated in [94], where the vectors such as velocity are remapped in frame-invariant way, leading to perfect symmetry preservation on conforming grids and a substantial reduction of mesh imprint on others. For an example showing cyclic remapping of a point-symmetric problem on a structured quadrilateral (logically rectangular) mesh, see Fig. 11.

Definitely worth mentioning among modern remapping methods is the Multidimensional Optimal Order Detection (MOOD) strategy [20, 58, 8], which also combines high-order and low-order reconstructions by precalculating candidate solutions, classifying the cells as valid (good) or troubled (bad), and *a posteriori* deciding which of the candidates is safe to be used in the latter. Although MOOD was created quite recently, it has since already been used in many contexts, formulations and applications - refer to the impressive lists in [82, 81].

3.6 Example Applications

The main application area of the Lagrangian and ALE calculations in our research group² are the simulations of the laser-target interactions. Closing the hydrodynamic equations by a suitable equation of state and supplementing the model by mechanisms such as laser absorption, heat conduction, separate treatment of ions and electrons or material mixing, we obtained a powerful tool to simulate experiments aiming at the Inertial Confinement Fusion (ICF) or laboratory astrophysics. After verifying and calibrating the simulation codes against experimental data, for example by comparing the post-processed spectra or the dimensions of craters in the targets, we can use them to study the effect of varying particular simulation parameters, such as the laser beam intensity and profile or target material and structure, to design new experiments while saving time and valuable resources.

One tool to do this is Prague ALE (PALE) [54], which is a twodimensional staggered ALE code being maintained and continually developed by the department's staff in collaboration with students and in partnership with researchers from facilities such as PALS (Prague Asterix Laser System) or ELI Beamlines (Extreme Light Infrastructure). Especially in the cylindrical (r-z) regime, it has been successfully used for validation, interpretation and prediction of data from real experimental campaigns. This can be very helpful to design the targets consisting of various material layers or having certain structure, for example containing low-density foams in order to achieve smoothing of laser intensity modulations [51] or accumulate high density of thermal energy in order to accomplish nuclear fusion ignition [37]. We also used the PALE code

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Figure 12: Generation of collimated plasma jet outflows by annular laser beams. Left panel: Various radial intensity distributions of beams given by analytical functions (top) and calculated from a real experiment at PALS (bottom). Right panel: Evolution of electron density for selected beam profiles [42]

to assess the idea of achieving simple and reliable generation of plasma jets with tunable parameters by using plasma beams with various spatial profiles [42]. To clarify observations from an experimental campaign at PALS, we performed simulations proving that the irradiation of a planar target using a laser beam with annular profile may lead to the formation of a collimated plasma jet, which is not the case when a Gaussian pulse with the same energy is used - see Fig. 12 for examples. This work turned out to be of interest not only to the ICF community pursuing one of the fast ignition concepts (searching for parameters suitable for the ignition of the pre-compressed fuel), but also found audience among astrophysicists. The actual interaction of plasma jets with solid surfaces has been studied in [72, 71].

Numerical methods developed in our research group have been also used in the framework of other complex simulation codes. As it was already mentioned earlier, several recently published works leveraged our library HerEOS [101] for thermodynamically consistent evaluation of realistic equations of state such as SESAME [63] or QEOS/FEOS [69, 28]. It



Figure 13: Simulation of a laser pre-pulse. Profiles of density and electron temperature obtained with various EoS applied and compared using the HerEOS tool [101]

has been used as a module with the PETE (Plasma Euler and Transport Equations) code [40], which includes the non-local transport hydrodynamics for laser plasma modeling and is constructed on the high-order curvilinear finite elements library MFEM [23]. Fig. 13 demonstrates how diverse results were obtained by employing various equations of state in a series of simulations for experiments with the pre-pulse of the LULI laser system in France.

Another particularly interesting simulation was performed by M. Holec as a part of an experiment at the OMEGA facility in Rochester, USA, and the follow-up deep analysis of how the EoS describes warm dense matter conditions created by a hydrodynamic shock in polystyrene foam [30, 29]. In the experiment setup sketched in the left panel of Fig. 14, a multi-layer target, consisting of a plastic ablator, an Aluminum pusher with gold coating, and C₈H₈ polystyrene foam, was irradiated by fifteen laser beams overlapped to give a planar square drive. The laser-driven shock gradually propagated through target layers into the foam, where the actual shock velocity was measured experimentally. The thermodynamic conditions in the shock wave traveling through the C₈H₈ foam were studied with suitable diagnostics and the shock velocity was measured by an interferometer system by detecting shock break-out times across four $40 \,\mu m$ steps manufactured on the back side of the target. The right panel of Fig. 14 shows the simulated evolution of density in the form of a colormap overlaid by some additional data. The simulated shock velocities are in very good agreement with experimental measurements given above. The following Hugoniot jump condition analysis revealed that at every moment of the shock propagation, the simulated shock velocity was in excellent



Figure 14: Velocity of laser-driven shock in C_8H_8 foam at OMEGA laser facility. Left: schematic picture of the multi-layer target. Right: result of the PETE simulation using SESAME EoS interpolated by HerEOS [101]

agreement with the shock velocity given by the SESAME thermodynamic jump conditions. Moreover, signs of a finite preheat due to non-local electron transport were observed in the simulation as well as in the experiment [30, 40, 41]. This clearly shows the synergy between the real experiments and hydrodynamic ALE simulations: the calculations not only help to set up the experiment and double-check the results, but also can provide deeper insight into the physics of the problem, which might be hard to observe and measure directly. On the other hand, experimental data are a great opportunity to validate the simulation code and assess the suitability of the physical and mathematical model used.

4 Current Research and Future Prospects

One of the current research topics of our team (Computational Physics Group, CTU, FNSPE) are the cell-centered Lax-Wendroff (LW) schemes on irregular and general polygonal grids. The classical LW scheme is usually written in Richtmyer's two-step formulation [73], that is, in the predictor-corrector form, where the predictor is the same as in the twostep Lax-Friedrichs (LF) scheme. It can be interpreted as starting from the nodal values of conserved variables at the old time level, which have been obtained for a given node as an average of the values in its connected cells, weighted by the masses or volumes of these cells or their parts. Using the concept of subcells, each of which is (in the 2D case) a quadrilateral given by the cell's center, one of its vertices and the midpoints of the two cell edges attached to this vertex, one can define a dual cell as the collection of all subcells attached to a node. Then, in the classical LF predictor, the nodal value (state) of a variable is defined as a mass- or area-weighted average of the corresponding subcell values over the dual cell. Unfortunately, on highly non-uniform meshes the standard Lax-Wendroff scheme with this Lax-Friedrichs predictor produces serious oscillations, which render it useless. In [96], Wendroff and White suggested two schemes using different predictors, making the methods robust and accurate even on such meshes. These predictors can be interpreted as approximating the nodal states by weighting with inverse values of subcell volumes. It is easy to show, that in one dimension and on rectangular 2D grids with generally irregular spacing, replacing volume weights by their inverse values corresponds to replacing piecewise constant reconstruction in cells by piecewise linear (in 1D) resp. bilinear (in 2D) interpolation from cell centers to nodes. Being aware of this fact, in recent paper [57] we followed up on [96] and studied the convergence of the suggested onedimensional schemes, applied them to a full system of conservation laws, further extended the methods to two dimensions and proved their secondorder accuracy.

The potential of inverse weighting on irregular meshes has also been demonstrated in [31], where it was applied in the recently introduced cellcentered Lax-Wendroff HLL (Harten-Lax-van Leer) hybrid scheme for Lagrangian hydrodynamics [32]. While the actual inverse weighting has been proposed already in a paper primarily dealing with the extension of [32] to r-z geometry [33], where its effect has been shown on structured grids (logically rectangular and equi-angular polar), in [31] we implemented it on general unstructured polygonal meshes, where inverse area weighting in predictor is not easily interpreted as a bilinear interpolation from discrete cell-centered values to nodes, but it turned out that even here the resulting scheme is viable. Currently, we are studying and practically testing also other types of nodal weighting.

Other ongoing topics related to hydrodynamic ALE simulations are including extensions of the model to involve elastoplasticity, more sophisticated multimaterial calculations, material mixing, structured targets, radiation transport, new implementations of laser absorption, etc. Very promising is also the research involving the Voronoi tessellations in twoand three-dimensional mesh generation, rezoning and remapping.

Most of the new ideas are being tested and unraveled in the framework of common Lagrangian and ALE simulation codes being continuously developed and maintained at our department by staff members and students pursuing their bachelor's, master's and doctoral degrees. Besides the already mentioned staggered ALE code PALE [54] for structured 2D meshes, there exist further research codes involving alternatives such as cell-centered discretization, Eulerian calculations and the use of general unstructured polygonal meshes, with the outlook of advancing to three dimensions and maybe incorporating our own implementation of high-order curvilinear mesh elements. This ecosystem of codes allows its users and developers to test and compare their new ideas and methods in various environments, with no need to write dedicated codes from scratch. For the students, this is a great opportunity to experience hands-on science, develop their professional skills and prepare for collaborative work in (preferably scientific) teams after their graduation. For the staff members, this collaboration is a source of new ideas, inspiration and (sometimes also) energy radiating from the students due to their enthusiasm.

5 Conclusion

This presentation reviewed selected results of research on which its author collaborated in the course of last ten years. The primary purpose of all these projects was the improvement of numerical methods to be used in the framework of Lagrangian and ALE hydrodynamic simulations, especially for the study of laser plasma interaction and high energy density physics. For particular aspects of the ALE methodology, a brief overview of popular and state of the art methods was given, with special focus on the context and contributions of the publications featured in the author's habilitation thesis [84].

The topics and novel or improved methods suggested in these papers include artificial viscosity for Lagrangian schemes, Hermite interpolations for thermodynamically consistent treatment of the equation of state, symmetry preservation (of symmetric problems) at all stages of the indirect ALE algorithm, mesh adaptation strategies that are effective and driven by the solution, and a series of methods for flux-corrected remapping. A little sample of practical applications of the resulting simulation codes was given to illustrate how the new methods can contribute to a better evaluation and understanding of complex real experiments or their parts, as well as to the design and setup of new ones.

Finally, some of the ongoing research topics were presented, related scientific and educational plans for near future described, and long-term objectives mentioned. However, the latter was rather meant to specify the author's current scope of interest, as he is always eager to learn from the others and thus open to new ideas, collaborations and research challenges.

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