High Performance Algorithms for Multiphase and Multicomponent Media

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Introduction. Although the main problem of multicomponent media dynamics still remains large difference of characteristic values of the processes, there are some indications, that it can very effectively be solved by the change of dynamic parameters, thus quasi-diagonalzing the rates of processes matrix. To overcome the difficulty of representing flow parameters in new variables one can use such procedure to all dynamic variables, not only with large difference of characteristic time. With the populations such approach is straightforward and intuitively clear, and it has support with a lot of effective examples in quantum mechanics. It is more interesting to do the same with flow variables. It is difficult to do this with standard representation of transport equations, but one can more effectively use the conservation laws in moving coordinates frame. In such a case one has simpler representation for derivatives in discreditized representation and thus a lot of possibilities for speed-up of computations. For efficient numerical implementation tensor representation in two coordinate systems (global and moving) is used. Proposed approach takes possibility to use explicit numerical schemes that result in natural parallelism of numerical procedure.

Mathematical Foundation. It is easy to understand bases of the proposed algorithm on the example of the evolution equation of the type

$$idu/dt = Pu, \tag{1}$$

with $\boldsymbol{P}$ being some operator, which we will suppose to be Hermitian. Any standard approach normally will transform it to the linear system of ordinary differential equations of the type

$$id\vec{v}/dt = \boldsymbol{P}\vec{v}, \tag{2}$$

with $\vec{v}$ being the large vector and $\boldsymbol{P}$ being symmetric matrix. The problem is not difficult for any size of $\vec{v}$, if $\boldsymbol{P}$ is almost diagonal, but for many important situations it is not the case. From the point of view of the theory of dynamic systems large nondiagonal members in $\boldsymbol{P}$ means bad choice of representation for Eq.(1), although often such representation is forced by physical considerations.

Usually it is not difficult to find the transformation, which will make $\boldsymbol{P}$ quasidiagonal, some of the beautiful approaches in the theory of nonlinear equations can have even natural physical background. At the same time some problems may cause the reverse transformation to original variables.

To find out what should be a correct dynamical approach let us look at one dimensional model that can be represented in simple form

$$u_t + uu_x - \mu u_{xx} = H(u,x),$$

with H being functional of flow parameters. Brilliant analyses of Prof. Ladyzhenskaya (1972) [1] on solution and uniqueness of this equation shows, that main problems can come from second term of lhs. If H can be represented as gradient of some functional, the problem can be solved by representing u as gradient of some v and integrating this equation one time. Actually exactly in such a way we can introduce famous Coul-Hopf transformation

$$u = -2\mu \frac{1}{v}\frac{dv}{dx}$$

that can linearize our equation in u in case of H being gradient of some functional. In general case it is not the case and we face all the problems of Navier-Stockes approach. One can imagine representation

$$K \equiv \frac{d}{dx}\left(\frac{d}{dx}\right)^{-1} K$$

and try to extract some sense from inverse operator of d/dx. It is very often done in quantum field theory, sometimes successfully, sometimes not [2]. The reason is non uniqueness of such operator. To give to it some foundation it is possible to return to foundation of hydrodynamic equations from kinetic ones and to obtain the way of regularization of such procedure [3]. In such a way one can come to new dynamical picture that we can illustrate on simple model.

Proposed approach. Here we shall study the problem on the base of one dimensional model, for which it is easy to make reverse transformation.

Let us assume, that *c* is any dynamical parameter and we shall discreditize it changing space coordinate x to index j. The system of transport equations, describing the flow in this one dimensional systems, consists in realistic cases of thousands of equations of the type

$$dc(j,t)/dt = I(j-1,t)I(j,t), \qquad (3)$$

with I being the current of this dynamic parameter in index space in and out of discreditization cell. It is always possible to present I as linear form of c, thus representing r.h.s of (3) in a way $I(j,t) = K(j,j+1)c(j,t) - K(j+1,j)c(j+1,t)$, where K may be a complex functional of all dynamical parameters.

The problems with Eq.(3) actually come from two factors — there are large nondiagonal members, corresponding to important physical transitions, and values of $I(j,t)$ are very large with difference between them in r.h.s. of Eq. (3) is relatively small. The situation becomes dramatic if you start integration with thermal equilibrium, when all *I*'s are equal.

To overcome those difficulties it is useful to introduce new variables $f(j,t) = c(j+1,t)/c(j,t)a(j,t)$ with $a(j,t)$ being the ratio of functionals $K(j,j+1)$ and

$K(j+1,j)$. f's are so called slow variables, which become constants at equilibrium conditions. The equations for f's are

$$df(j,t)/dt = \tilde{R}[f(j,t)] + H(j,t)f(j,t) + S(j)f(j,t), \quad (4)$$

with $\tilde{R}$ being the quadric term, that is diagonal in j, H is the source term, proportional to external fields, and S is the source of dynamical parameter change, the only term, that is nondiagonal in $f(j,t)$. The main advantage of Eq.(4) is, that not only the sum of three terms in r.h.s. (4) is small, but they are small separately and it is easy to determine their relative values beforehand. Moreover, it is important, that the major contribution in r.h.s. of (4) is diagonal that opens interesting opportunities for parallel algorithm.

Such notation makes it possible to rewrite numerical schemes in tensor form. Tensor mathematics naturally embedded in the finite- operation in the construction of numerical schemes.

Stages of the computation. The traditional computational scheme for the above described approach is already realized as a computer code for Power clusters and includes following phases:

1. Functional constants *K* computation,
2. Functional constants *K* parametrization,
3. Approximate system evolution,
4. Corrections for exact system evolution,
5. Populations and averages computations.

Since even in this new approach, the whole computational problem is prohibitively time consuming, in practice it is separated into three stages:

I. Stages 1 and 2,
II. Stages 3 and 4,
III. Stage 5

And usually it is realized on different systems. The stages I and II are the most difficult ones. We are not discussing here the realization of stage I, which is more or less standard.

It is enough to note, that the results of stage I are the input for stage II, and thus should be realized as Data Base, or Knowledge Base with pertinent gate to the system, realizing stage II. What we are proposing here is to use absolutely parallel nature of the algorithm, discussed above to realize substantial part of the computations in Items 3 and 4, which are actually reduced to the solution of huge amount of Ordinary Differential Equations, connected only by initial data. For that purpose we split this algorithm in separate blocks and realize it on different systems.

Important Example

For illustration of proposed approach we have taken thermal wave in mixture He-HF in one dimensional flow with initial temperature difference between plates of 1300K. The reason of this is obvious. There are not so large gradients involved and we can prepare and keep all necessary data for functional constants *K* on the same system. So we can skip the large part of Grid infrastructure

and concentrate only on peculiarities of computational algorithm. To check the real advantages of our approach and see possibilities for its migrating to Grid infrastructure we test it on a cluster with slow links.

To simulate this flow we must solve standard equations (3). It is very effective demonstration, since number of discretization boxes, which should be taken into account, is of the order of 80 with such temperature spread, so one needs not much time for convergence of flow solution. Computation was done on 8-processor linux cluster with slow 2Gb links to simulate importance of communications between computational processes.

The complete simulation of initial problem took about 20 min. The use of relaxational system (4) instead of (3) reduces that time to 2.4 min.

In this case it is possible to increase essentially effectiveness of computing procedures through:

1. Natural parallelization of the computation process;
2. Possibilities of adaptive correction of mesh area depending on features of the problem;
3. Dynamic reconstruction of solution in accordance with fluid currents transformations in time.

Conclusion. It is known that traditional approach to numerical solution fluid dynamics problems is most often reduced to application of implicit schemes. The described algorithmic approach, first of all because of the proposed splitting of the solution on physical processes, gives the chance of application explicit numerical schemes. It is even more interesting to see how all this arrangement works for more complex hydrodynamic flows, but that we will show in our next paper.

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References

[1]. G.B. Whitham. Linear and nonlinear waves. JOHN WILEY and SONS, 1974.
[2]. P. Ramond. Field theory. A modern primer. The Benjamin Cummings publishing, 1981.
[3]. V.Ya. Rudyak. Statistical theory of dissipative processes in gases and liquids (in Russian). Nauka, 1984.