Hot (summer) ideas on seismic finite-difference methods

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State of the art

We currently use several explicit finite-difference (FD) schemes for seismic wave propagation (Zahradník, Moczo and Hron, 1993). They solve the time-domain elastodynamic equations in the displacement components. Common properties of the schemes are: regular square grids, 2D isotropic media (polygonal block structures), flat free surface, P-SV and SH waves, excitations by a vertically incident plane wave, or a body-force source inside the FD region, no absorption. Where applicable, the spatially constant absorption is employed with a causal or non-causal quality factor Q(f) by the *a posteriori* correction of Zahradník, Jech and Moczo (1990). All the schemes are in a heterogeneous formulation (justified in Zahradník and Priolo, submitted), but they differ in the way how the material parameters are treated. One of our SH schemes is 4th-order accurate in space and 2nd-order in time, $O(h^4, k^2)$. The other SH schemes, and all P-SV schemes, are $O(h^2, k^2)$. One exception was an $O(h^4, k^2)$ P-SV scheme of Zahradník and Hron (1992) which is no more in use by us as it was shown violating the traction continuity at material discontinuities. The flat free surface is treated by the vacuum formalism, justified in Zahradník, O'Leary and Sochacki (1994). The exception is a P-SV scheme modified from Kummer et al. (1987), for which the vacuum formalism violates the free-surface condition, and a special scheme of Moczo is used (see Appendix of Zahradník, Moczo and Hron, 1993).

Objectives

Strongly required are the following innovations: Better $O(h^4, k^2)$ P-SV schemes, hereafter simply called 4th-order schemes. Schemes treating non-planar free surfaces. Schemes more efficiently treating the media with both very low and very high velocities in a single model. Schemes treating a spatially varying absorption. Schemes allowing realistic excitations by a point or finite-extent source, located outside the FD region.

The 4th-order accuracy everywhere

As shown in Zahradník, Moczo and Hron (1993), the scheme of Kummer et al. (1987) has good properties at internal discontinuities. Anyway, its accuracy at the discontinuities is not better than $O(h)$. Several modifications of this scheme, keeping $O(h^4)$ everywhere (including the internal discontinuities, and the flat free surface), was recently developed

theoretically by Chroust (diploma theses, unpublished). His schemes differ of each other in the way how the treatment of the internal and free-surface points is combined, and how the non-reflecting (Stacey's) boundaries are employed. In general, the schemes are highly complicated, with many arithmetic operations per a grid point. Their dispersion properties in heterogeneous media have not yet been investigated. Therefore, the efficiency of the schemes is not clear.

Despite the great sophistication of the new schemes, limited numerical experiments performed till now have indicated only very little differences in synthetic seismograms, with respect to those computed by previous simpler schemes. Moreover, even relatively simple models have often suffered from unconditional instabilities. Presently it seems that the instabilities were mainly due to the combination of the new schemes with the Stacey's nonreflecting boundaries. This result is interesting as the Stacey's conditions have been often reported in literature as working well. However, Moczo (personal communication) also mentioned problems when plugging one of the Stacey's conditions into his 2nd-order scheme.

Partial conclusion. Alltogether, our preliminary results with the new 4th-order schemes are not very encouraging. It seems necessary: (i) to try other nonreflecting conditions, (ii) to clarify the accuracy improvement (if any), and efficiency, and (iii) to carefully decide whether to continue in this work or not. Note that discussed here is something very different from what is called 4th-order scheme in literature, where the accuracy order at discontinuities is actually lower than the 4th. In this light it cannot be ruled out that the requirement of the 4th-order accuracy everywhere is too ambitious, and, because of its high complexity, it very often numerically fails for various reasons. This pessimism comes from the independent recent result of Zahradník (submitted) who compared two 2nd-order P-SV shcemes, a complex and a simple one, found nearly identical results, but very frequent instabilities with the complex one.

Integration-approach schemes

There is a chance that certain schemes permit less problematic 4th-order generalizations than the scheme discussed above, perhaps including the case of the 4th order everywhere. Let's discuss, for a while, the velocity-stress method. Its 4th-order version (Levander,

1988) is successfull, but it is obviously no 4th-order accurate everywhere. The stability is most likely due to the tricky staggered grid. However, staggering is similar to our displacement schemes: although the stress components are not used as unknowns in our schemes, the stress-related terms (e.g. $\mu\frac{\partial u}{\partial x}$) are always approximated at locations between the displacement grid points. Therefore, the main difference is only in the treatment of the material parameters (local values in the velocity-stress method, and geometrical averages in our). For these reasons we probably cannot expect less complications with the velocity-stress method when trying to keep its 4th-order accuracy everywhere.

It may be that major problems with higher-order generalizations occur due to the double differentiations typical for most FD shcemes: the first one in computing the stress terms, like $\mu\frac{\partial u}{\partial x} = g$, and the second one in computing $\frac{\partial g}{\partial z}$, etc. Therefore, we hypothesize that less problematic might be the schemes avoiding the second differentiation. That is the case of the schemes based on the integral equations of motion, like in Zahradník, O'Leary and Sochacki (1994). Denoting the stress tensor by τ, by the Gauss theorem we get $\int_V Div\tau = \int_S \tau$, which, in the 2D case, transforms to a contour integration at an element volume of the FD grid (Fig. 1). The traction-continuity condition can be automatically satisfied at a discontinuity Σ, but it may be later violated when improperly approximating the line integral at the remaining (rectangular) parts of the integration contour. Some of the approximations even yield instabilities (Zahradník, submitted).

Another reason for preferring the integration approach is the simplicity of the free-surface approximation by the vacuum formalism, which is quite natural in that approach. By far not all FD schemes permit the vacuum formalism, as already mentioned with the Kummer et al. scheme.

Partial conclusion. Our working hypothesis is as follows: The integration-approach (hereafter IA) schemes should be better than the conventional differential-approach ones, because IA is avoiding one of the space differentiations. However, a good deal of work remains to be done on a proper approximation of the corresponding contour integrals, mainly if a higher-order accuracy is desired.

Irregular grids

When applying the vacuum formalism to a free surface, the geometrically averaged

material parameters become zero-valued wherever an arbitrarily small part of the grid leg is above the surface. This yields an apparent distortion of the surface form. We expect this fact to seriously limit the applicability of the vacuum formalism to non-planar free surfaces at regular grids. A partial solution to this problem is the grid refinement in the surface parts of the model. Another reason for the grid irregularity comes from models with very soft sediments overlying hard rocks. From a large variety of possible grids we prefer the irregular grids of Moczo (1989), regular in x, and irregular in z (Fig. 2). Their advantage is in simplicity; no interpolation is needed at the contact of the unequal grid steps.

Partial conclusion. We suggest to organize the work in two lines: (i) New IA schemes of 4th-order accuracy on regular grids, (ii) 2nd-order IA schemes on irregular grids, including non-planar free surfaces.

Small time steps

Having an irregular grid, a relatively very small space step will be used at the non-planar surface, and in the low-velocity regions. The stability condition, therefore, will imply a very small time step. Realistic models will require about 10^4 time levels to be computed. This is not only time consuming, but it increases the potential of numerical problems at the nonreflecting boundaries, too. Moreover, as a single time step k applies for the entire FD model, including the regions of large velocities (hence large h), we will face the problem with low k/h ratios, well known for their poor dispersion properties.

Partial conclusion. The requirement of too small time steps stimulates us to think about another alternative, i.e. the FD solution in the frequency domain.

Frequency-domain FD method

Obvious advantages of the frequency-domain FD method (hereafter FDFD) are: (i) minimization of the grid dispersion without the need of higher-order schemes, simply through spatially irregular grids, adjusting the step sizes correspondingly to the local velocities, and (ii) a possibily variable coaresness of the grids for different frequencies (Korn, 1987). On the other hand, although the 2nd-order schemes keep the resulting matrices sparse enough, problems can be expected to arise from the size of the resulting algebraic systems for P-SV waves. Maybe that some iterative methods could be used in which the

first iteration is not a formal one, but it is determined from a cheap (low-order, regular grid) time-domain FD method.

Any FDFD automatically implies the complex-valued displacement. It is not because of the involved differential operators, but due to the source time functions. Once the adventure of the complex arithmetics is entered, there is only little additional work to employ the absorption effects through the complex-valued material parameters (Korn, 1987). A spatially varying quality factor $Q(f)$ would become possible. This is another strong argument for trying the FDFD, because the time-domain FD methods with absorption (Emmerich and Korn, 1987) are time and memory consuming.

Partial conclusion. The time-domain FD methods need higher-order space operators and/or irregular grids. The irregular grids yield impractically small time steps. Including absorption in the time-domain FD scheme is both memory and time consuming. The frequency-domain FD methods permit low-order space operators at spatially irregular grids. Large complex-valued algebraic systems have to be solved, but the absorption is included at no axtra cost. To organize the work properly we should start with FDFD at flat-surface sedimentary sites, where the spatially varying absorption is urgently needed. The topographic problems should perhaps continue with the time-domain FD methods, as there is usually no mixing of very low and high velocities in a single model, and also the spatially constant Q(f) is often applicable by means of the *a posteriori* correction.

Excitation

Obviously, no problems arise with excitations by body-force terms, both in the time- and frequency-domain FD methods. However, also the excitation approach by Alterman and Karal (1968) has been widely applied in the time-domain FD methods. Let's call it A-K excitation, and discuss some of its properties. The wavefield is represented as a sum of a known part, u^k, and a remainder, u^r: $u = u^k + u^r$. The FD region is divided in two subdomains, A and B (Fig. 3a). The FD solution is performed for u and u^r in A and B, respectively. The A region includes the line a, and similarly for B and b. While updating u at line a we obviously need u at line b, too (Fig. 3b). This is found from u^r, computed by the FD method at line b, adding u^k to it: $u = u^r + u^k$ at line b. We proceed in a similar way when updating u^r at line b, employing the knowledge of u and u^k at line a: $u^r = u - u^k$

at line a.

All this is well known. Nevertheless, less recognized is the fact that the representation $u = u^k + u^r$ is not unique.In different methods, u^k and u^r may have a different meaning. For example, when exciting a local 2D structure by a plane wave, u^k is the *incident* wavefield, as a rule. No reflections from the free-surface are included in u^k. Therefore, u^r becomes relatively strong. Otherwise, u^k may describe all the 'background' effects that would exist in the absence of the local 2D structure, including, for example, the free-surface reflections. Then, u^r would be relatively weak. This would be the case of the excitations (input motions) provided by independent numerical methods. The 'background' solutions u^k may be generated for simple media, say the horizontally layered media, with a line or point source, using, e.g., the modal summation, or the discrete-wavenumber method. Nevertheless, u^k generated for 2D or 3D 'background' media by, e.g., the ray method are also possible. Typically, the durations of u^k including all the 'background' effects (perhaps even surface waves) is much larger than that of u^k describing a single incident plane wave only. Saving any numerically prescribed u^k for long excitation lines, and large durations, is memory consuming a lot.

Thinking about efficient hybrid methods it should be emphasized that two excitation lines, as in Fig. 3a, are the case of 2nd-order FD methods only. Any 4th-order method needs four lines (as already successfully implemented in our 4th-order SH code). That requirement is very impractical, not only for the memory needed in the FD method, but also for the computing time needed when providing the input motion. Even more demanding would be the excitation lines surrounding the studied 2D objects, as in Fig. 3c. The reasons for such excitation lines are discussed by Zahradník (in preparation).

Partial conclusion. The A-K excitations become impractical with higher-order FD methods. This fact again stimulates thinking about the FD solution in the frequency domain, where 2nd-order schemes are likely sufficient.

Excitation in the frequency domain

It is to clarify whether the A-K excitation, originally developed for the time-domain methods, is applicable also in the frequency domain. We prove that it is applicable, because it is nothing but a kind of the body-force source term. To show this, let's consider the

simplest 1D propagation: $S(u) = T(u)$, where S and T are the space and time operators, respectively. For the 2nd-order scheme, $S(u) = (u_{L+1} - 2u_L + u_{L-1})/(h^2)$. When u_L is updated at line a of Fig. 3b (subscipt L), u_{L+1} from line b is needed: $u_{L+1} = u^k_{L+1} + u^r_{L+1}$. The substitution of this representation of u_{L+1} into $S(u)$ yields

$$\frac{u^r_{L+1} - 2u_L + u_{L-1}}{h^2} + \frac{u^k_{L+1}}{h^2} = T(u_L),$$

which can be written as

$$S(\tilde{u}) + force = T(u).$$

We have got the same operator S as above. The only difference is that the operator has been applied now to something (denoted $\tilde{u}$) which is of a different meaning in regions A and B, i.e., u and u^r, respectively. The excitation enters the scheme as the body-force term determined by u^k. As the FDFD excited by a body force should not present difficulties, we do not see principial problems in applying the A-K excitation in the frequency domain.

Partial conclusion. The A-K excitation is, in fact, equivalent to a body-force term. We should try to employ it in a FDFD method.

Deffects: a new excitation method

Memory requirements of the A-K excitation stimulate thinking about another excitation method. We speculate about body-force terms spatially more concentrated than on lines a and b in Fig. 3. As in the indirect boundary element methods (e.g., Pedersen et al., submitted), the wavefield scattered by a 2D object should be described by body forces distributed along the boundary of the object. However, unlike the boundary element methods, where the body forces are computed by the Green function formalism, and the displacement/traction continuity conditions, we should look for a purely numerical determination of the body forces.

Let $u = u^k + u^r$, as in the previous paragraph, with u^k being the wavefield in absence of the local 2D object. Let $S(u) = T(u)$, with the space and time operator S and T, describes the problem with the 2D local object, including its excitation by a distant source and no body forces (Fig. 4a). Then, our intention is to look for such body forces (Fig. 4b) that

$$S(u^r) + force = T(u^r).$$

Because of linearity of S and T, the equation $S(u) = T(u)$ can be written as

$$S(u^r) + S(u^k) - T(u^k) = T(u^r),$$

which is already in the desired form, while $S(u^k) - T(u^k)$ is playing the force-term role.

As S represents the 2D problem with the local object, while u^k solves for a simpler problem without the object, the body-force term $S(u^k) - T(u^k)$ does not vanish, in general. Similarly to multigrid methods, we perhaps can call this term 'deffect', i.e. the deffect of the known solution u^k on the 2D problem. Once the deffect is known, it provides the body-force necessary for the FD computation of the remaining part of the wavefield, u^r. It is likely that computations of the deffects are possible, and, moreover, relatively easy. Actually, once we know u^k for a single FD stencil (i.e. for a few grid points around the studied one, both in space and time), the deffect can be computed by the application of the standard FD version of the operators S and T. This, of course, can be performed for any isolated grid point, without complete stepping through the entire space and time grid.

We expect (perhaps erroneously) that the deffect is significant in spatially localized regions. For example, for shallow sedimentary basins, we expect the most significant deffects close to the edges of the basin. It this is the case, the FD excitations of the basins would be highly simplified as compared to the A-K method.

If interested in the applications in which the most valuable are the first arrivals only, another advantage of the described excitation would be the possibility to combine it with the speed-up method of Vidale (1988). The first-arrival time is computed by an independent method, separately of the FD program. Then, for any grid point, the FD computations are performed in a prescribed vicinity of the first-arrival time only. The computer program for this purpose has been already developed and tested by Kvasnička and Zahradník (unpublished), but it has not yet been widely used.

Partial conclusion. We suggest to numerically investigate the so-called deffects of the 'background' solutions (the ray-method, or the discrete-wavenumber method solutions) on 2D problems with local objects. As far as we know, this subject is new, and offers interesting opportunities in defining the body-force equivalents to the scattered wavefields.

We assume that the deffects might provide an alternative to the A-K excitation, thereby serving to build-up efficient hybrid methods.

Hybrid method

For computing the excitation of the FD models, i.e. u^k introduced above, we have decided to employ the discrete-wavenumber (hereafter DW) method of Bouchon (1981). The computer program, written and provided to us by O. Coutant (Grenoble University), has been already implemented at our PC. Perhaps of interest might be to mention a troubling period of the implementation, when we were obtaining completely wrong results in some runs, and quite perfect results in the others. Of course, the problems were not due to the program, but due to our customization of the Fortran Power Station compiler (employing the speed-optimization option). For reasons not clear to us this compiler option, in a certian combination with the others, sometimes fails.

Main reasons for choosing the DW method have been the following: The DW method computes the complete wavefield, including all interference waves (e.g. surface waves) that occur in a horizontally layered halfspace with a true 3D (point) source of an arbitrary focal mechanism, possibly also an explosion. Near-field effects are included, too. The spatially varying absorption is considered by means of the complex-valued material parameters.

Let's also mention some technical features of the DW method. It is a two-step method. First, the Green tensor is computed in the frequency domain, and, in the second step, the source moment tensor and its time function are employed. Finite-extent sources are modelled as a sum of point subevents, including their (possibly) different focal mechanisms and time shifts. The slip functions of the subevents do not differ of each other. The source and receiver cannot be located at the same depth. This limitation is not too severe for the earthquake ground-motion simulations, because the sites investigated by the FD method rarely reach depths larger than one kilometer, while the crustal earthquakes are usually deeper. It is, however, a severe limitation for the explosive sources, usually located at the surface, as well as the receivers. Otherwise, no technical problems arise when computing DW solutions for a single source and many different distances and azimuths, as needed in the A-K excitation. Of course, the DW computing time is proportional to the number of the receivers. It is likely that the excitation required by the FD method, i.e., for many grid

points, may be too impractical for the DW method unless a suitable spatial interpolation from less numerous DW receivers is employed. The requirement for interpolation in the DW solution is supported also by another reason: a single (time consuming) DW solution should be applicable to different FD models.

If the DW solution is used to excite the time-domain FD model, the time interpolation is needed, too. It is because the DW synthetics will typically be of a larger time step than required by the FD method. Moreover, long durations of the DW synthetics even for weak crustal earthquakes are to be expected. For this and the previous reason it might be better to couple the DW and FD method in the frequency domain.

A great advantage of the DW output and the FD solution in the frequency domain is that a pure transfer function of the medium can be computed, and used later with different time functions. In case of the finite-extent sources summed from the subevents this advantage becomes less pronounced. It is because the number of subevents also determines their size (and their durations). Therefore, with a given number of the subevents and a selected duration of the subevent, the ground-moion simulation can hardly be repeated with any other duration.

A small technical remark should be made in connection with the DW output/FD input. Let's consider the frequency domain. Any displacement component u at any frequency f is available on the frequency-domain DW output in the form of six independent Green function components $G_1^k(f),...G_6^k(f)$ for each subevent $k = 1,2,...N$. They have to be multiplied by six components of the source moment tensor $m_1^k(f),...m_6^k(f)$, and summed over the subevents:

$$u(f) = \sum_{k=1}^{N} \sum_{j=1}^{6} G_j^k(f) m_j^k(f).$$

As the DW program assumes different focal mechanisms a_j^k, and time shifts τ^k, but the same slip function $c(f)$ for all subevents, we have

$$m_j^k(f) = a_j^k e^{2\pi i f \tau^k} c(f).$$

Therefore, we plan to reorganize the frequency domain output as follows:

$$p^k(f) = \sum_{j=1}^{6} G_j^k(f) a_j^k,$$

$$g(f) = \sum_{k=1}^{N} p^k(f) e^{2\pi i f \tau^k},$$

$$u(f) = q(f)c(f).$$

This will allow to input the DW frequency-domain results with the already included focal mechanism, i.e. with a single $q(f)$ (instead of the six $G's$). Also, this representation enables to process the subevents ($p^k(f)$) separately of each other, if necessary.

If the FD computations are in the time domain, the standardly available time-domain DW output can be used, including the focal mechanisms of the subevents, their time shifts, summation, as well as the FFT. The time-domain equivalent of the transfer function of the medium, recommended above, is the impulse response. In our FD programs so-called pseudoimpulse responses are often computed, using finite but very short excitations. Numerical inaccuracies at higher frequencies are later removed when convolving with relatively low-frequency time functions. Therefore, we speculate about a possibility to do something similar with the DW excitation, too. Short DW synthetics would be advantageous also for saving memory in the A-K excitation. However, they are hardly possible: First, they are impractical for the DW method, because the short time functions have wide spectra, hence many frequnecies must be computed, making the DW simulation very time consuming. Second, as already mentioned, even with short time functions, the realistic crustal DW synthetics are often of a considerable durations due to multiples and interference waves.

Partial conclusion. The DW program, available to us from the Grenoble University, can provide the FD input both in the time and frequency domain (with a small reorganization in the latter case only). The choice between the two should come from our further experience with a frequency-domain FD method. More details on the intended hybrid DW/FD method, in particular new (2.5D) equations of motions to propagate the point-source DW solutions by the FD method, are given in Zahradník (under preparation).

Conclusion

Several innovations of the seismic FD methods have been suggested in this report. Some of them are of a technical character only, e.g. the irregular grid, the non-planar free

surface, and the new excitation lines. Their implementation and verification is a matter of programming and extensive numerical experiments. The others are more substantial, and will require a deep further research: the new 4th-order schemes, the FD schemes in the frequency domain, the new excitation method by the so-called deffects, and the new (2.5D) equations of motion for coupling the discrete-wavenumber and FD simulations.

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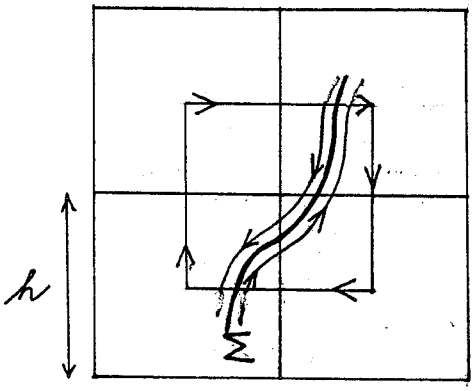

Fig. 1

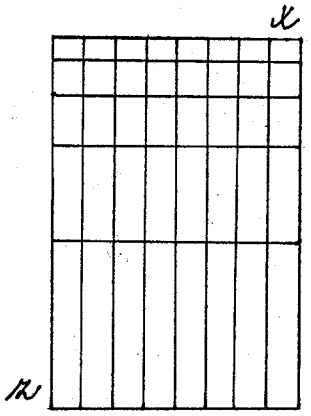

Fig. 2

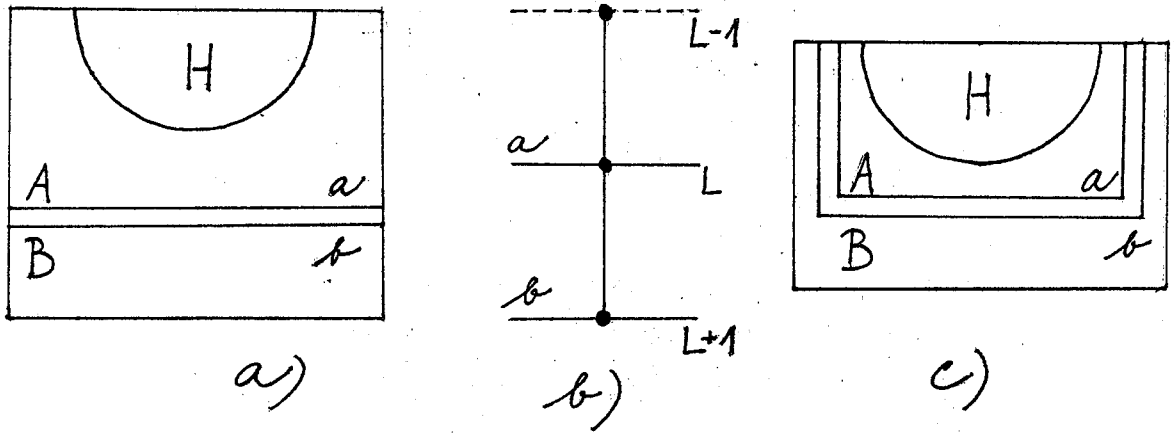

Fig. 3

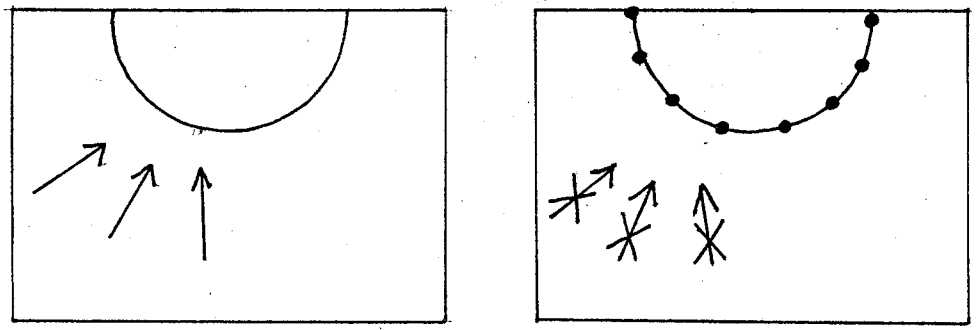

Fig. 4