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Institut für Neutronenphysik und Reaktortechnik
Projekt Schneller Brüter

Comparison of 3 Methods to Control the Leakage of Particles in a Monte Carlo Game

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Summary

Estimating with a Monte Carlo Code quantities which depend primarily on neutrons which have performed many collisions in a system becomes difficult when a high probability for neutron leakage hat to be faced. This may necessitate the use of track length truncation as a non-analogue method for treating neutron leakage, in order to improve the statistics for neutrons with high numbers of collisions. Kschwendt and Rief have shown the advantage of track length truncation (Expected Leakage Probability method, ELP) in estimating time-dependent neutron leakage from bare spheres (3). In this paper the same type of test problem has been investigated. It could be demonstrated that a considerable improvement over the ELP method can be achieved by combining track length truncation with a technique of angular biassing which promotes inward scattering in the immediate vicinity of all outer boundaries.

Zusammenfassung

Für Systeme mit hoher Neutronen-Ausflußwahrscheinlichkeit ist es schwierig, solche physikalischen Parameter mit der Monte-Carlo-Methode zu schätzen, welche überwiegend von den Neutronen bestimmt werden, die bereits viele Stöße im System erfahren haben. Es kann dann notwendig werden, die Track-Length-Truncation-Technik anzuwenden, d.h. die wahre Verteilungsfunktion für die Neutronen-Flugwege an allen Systemrändern abzubrechen und zu renormieren. Dieses Nichtanalog-Verfahren zur Behandlung des Neutronen-Ausflusses verbessert die Statistik für Neutronen mit vielen Stößen innerhalb des Systems. Kschwendt und Rief (3) konnten den Vorteil der Track-Length-Truncation-Technik, von ihnen ELP - Methode (ELP = Expected Leakage Probability) genannt, am Beispiel der Schätzung des zeitabhängigen Neutronen-Ausflusses aus homogenen Kugeln aufzeigen. In dieser Arbeit wird die gleiche Art von Testproblem untersucht. Es wird gezeigt, daß sich gegenüber der ELP-Methode erhebliche Verbesserungen ergeben, wenn man Track-Length-Truncation verknüpft mit solchen modifizierten Verteilungsfunktionen für die Streuwinkel, welche in der unmittelbaren Nähe von Systemrändern die einwärts gerichteten Streuprozesse begünstigen.

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Summary

Estimating with a Monte Carlo Code quantities which depend primarily on neutrons which have performed many collisions in a system becomes difficult when a high probability for neutron leakage has to be faced. This may necessitate the use of track length truncation as a non-analogue method for treating neutron leakage, in order to improve the statistics for neutrons with high numbers of collisions. Kschwendt and Rief have shown the advantage of track length truncation (Expected Leakage Probability method, ELP) in estimating time-dependent neutron leakage from bare spheres (3). In this paper the same type of test problem has been investigated. It could be demonstrated that a considerable improvement over the ELP method can be achieved by combining track length truncation with a technique of angular biassing which promotes inward scattering in the immediate vicinity of all outer boundaries.

Introduction

The starting point for this investigation is our intention to apply the Monte Carlo method, as a general tool, to the study of fast critical and subcritical assemblies. Some of these, e.g. GODIVA (1) and the SUAK assemblies (2), are small so that leakage has an important share in the neutron losses to be considered. Although some parameters of a fast assembly, such as the effective multiplication factor k_{eff}, are often determined by the complete energy spectrum of the neutrons, essentially uniformly, we are sometimes more interested in the sparsely populated low energy tail of the spectrum. This part of the neutron spectrum determines largely such important quantities as the effective prompt neutron generation time l_p and the Doppler effect. It must, therefore, be adequately covered by experimental and computational methods.

Obviously, pure Analogue Monte Carlo (AMC) is no efficient tool for estimating, in small fast assemblies, quantities which are determined by neutrons of lower energy. Even when the usual non-analogue collision kernel is applied for treating neutron absorption, the assumed high leakage probability leads to random walks with low average numbers of collisions. Starting at fission energy most random walks will end by leakage before getting into the lower energy region of phase space, which can be reached only through a large number of inelastic and elastic scattering collisions.

What we are looking for is, therefore, a modified transport kernel for the biassed random selection of flight directions and track lengths, which yields random walks with an increased number of collisions. Biassing thus neutron transport in the Monte Carlo game involves a redetermination of the neutron weight after each collision event.

The weights of neutrons in a specified volume of phase space may have been redetermined many times and show a smaller or larger dispersion, depending on the distance, in phase space, between the points of origin (= source coordinates) and observation and on the particular transport kernel. This dispersion of neutron weights increases the variance of estimates and can as a negative effect compensate to a considerable extent the positive effect of raising the number of passages of random walks through the specified volume of phase space. This is true, e.g., for the ELP-method recommended in (3). - A second criteria for the choice of a particular modified transport kernel is, therefore, that the dispersion of neutron weights should be low even after many collisions.

A third, often desirable, criteria is its general applicability. A modified transport kernel incorporated in a large general purpose Monte Carlo code should enable us to estimate, simultaneously, several parameters (k_{eff}, l_p, spectra, etc.) with tolerable statistical errors, instead of only a single parameter with a minimum error. With this aim in mind we have to discard attempts to implement a zero variance strategy, that would involve a specific source for the needed importance function and, thus, restrict the class of parameters which can be satisfactorily estimated at the same time.

Finally, the non-analogue technique implied by the modified transport kernel must be simple. If a sufficient number of collisions and histories must be processed in a given time, then at each collision only simple, fast-running algorithms may be invoked. Furthermore, Monte Carlo is a method in development, and only very simple techniques have some chance of being retained and adapted to advanced Monte Carlo strategies, such as self-optimization, that can be expected in future.

Model problem - time-dependent leakage

In order to test the performance of the modified transport kernels under consideration it was convenient to turn the attention from the original stationary, but energy-dependent problems towards very simple monoenergetic, time-dependent test problems, which are far easier to programme, but involve the number of collisions in a random walk in the desired, correct way. For this reason we chose as test-cases for 3 modified transport kernels two cases of a time-dependent leakage problem introduced in (3).

Case A: Consider a homogeneous sphere of outer radius

$$R_o = 3\,\lambda \qquad (\lambda = 1/\Sigma = \text{mean free path})$$

The only neutron process considered, besides leakage, is elastic scattering with a macroscopic cross section Σ. Scattering is assumed isotropic in the

lab system; but this assumption is not essential for any of the methods studied. The neutrons are monoenergetic with a velocity v.
At time t=0 source neutrons are injected at the center of the sphere and pursued till a final time

$$t_{max} = 15\ \lambda/v$$

The complete time interval is subdivided into 30 equal time channels of width

$$\Delta t = 0.5\ \lambda/v$$

For each time channel the mean number of collisions and of leakage events are to be estimated.

Case B differs from Case A only in a few respects, viz. the outer radius is smaller,

$$R_o = 0.7\ \lambda\ ;$$

the observation interval extends to

$$t_{max} = 8\ \lambda/v\ ;$$

the number of time channels is 40, and the channel width

$$\Delta t = 0.2\ \lambda/v$$

4 different Monte Carlo techniques have been applied to these test problems, viz. a form of Analogue Monte Carlo (AMC), the method of Expected Leakage Probability (ELP) recommended in (3), and two other non-analogue techniques (CAS, MELP) which combine the track length truncation scheme of ELP in different ways with angular biassing. An attempt was made to compare the methods on the basis of equal computer time. As this is possible only very approximately, in view of the unknown environment of any numerical technique in practical applications, the exact basis of comparison is explained below with each method.

Fig. 1 shows, on a logarithmic scale, the time dependence of the collision and the leakage rates for Case A. The points for each time interval have been obtained as weighted averages of the results from the 4 independent methods compared. Figs. 2 and 3 contain for each method the estimated relative errors associated with the collision and leakage estimates, in these figures only every second time channel has been included. These error estimates give us a clear indication of the advantage or disadvantage of each method in specified time regions.

In Figs. 4 - 6 the same information is contained for Case B.

Collision estimates, Analogue Monte Carlo (AMC)

In all 4 methods compared the collision rates have been obtained from a pure collision estimator. That means, after a collision at the position vector x and time t the actual neutron weigth W is registered as a contribution to the number of collisions in the time channel associated with the collision time t.

For AMC without absorption the neutron weight W is constant, W=1. In AMC after a collision at time t the flight direction vector Ω is selected from the isotropic angular distribution and

$$D(x,\Omega) = \text{distance from } x \text{ to the boundary in direction } \Omega$$

is computed. The expected value of leakage from the collision point x in direction Ω,

$$W \exp(-\Sigma D(x,\Omega)) \tag{1}$$

is registered for leakage in the time channel corresponding to the leakage time

$$t' = t + D(x,\Omega)/v \tag{2}$$

In AMC the track length d is then chosen from the exponential distribution

$$P_o(d) = \Sigma \exp(-\Sigma d), \quad 0<d<\infty \tag{3}$$

If $d<D(x,\Omega)$, new collision coordinates are computed, otherwise a new source neutron starts another neutron history.

To test AMC 200 000 collisions were processed for each test case, A and B.

Method of Expected Leakage Probability (ELP)

This method, recommended by Kschwendt and Rief (3), is a track length truncation method, which does not modify the angular part of the original transport kernel. The main difference from AMC is the selection of the neutron track length from an exponential distribution truncated at the boundary

$$P_1(d) = A^{-1}(x,\Omega)\cdot\Sigma \exp(-\Sigma d), \quad 0<d<D(x,\Omega), \tag{4}$$

$$A(x,\Omega) = 1 - \exp(-\Sigma D(x,\Omega)) \tag{5}$$

The newly introduced $A(x,\Omega)$ is the normalization factor for the truncated exponential distribution.

As a consequence of this modification the neutron weight W, which for source neutrons is $W_o=1$, changes in a collision at x with the new direction Ω from W to

$$W' = W\, A(x,\Omega) \tag{6}$$

The variable neutron weight W has to be applied in the estimation routines for collision and leakage rates, e.g. in Eq. (1) for leakage.

As the truncated track length distribution forbids direct, analogue leakage of neutrons, neutron histories end only when the time limit t_{max} is exceeded.

A comparison of the estimated errors obtained from AMC and ELP, cf. Figs. 2, 3, 5, and 6, shows for short observation times, i.e. in time channels of low order, an advantage for AMC, essentially due to the very large number of neutron histories which can be processed by AMC. For longer times and especially for the smaller system (Case B, Figs. 5,6) the advantage of ELP, as pointed out in (3), is obvious.

In this comparison for each ELP case also 200 000 collisions have been processed, i.e. for the change from AMC to ELP no additional computer time has been considered. In fact, for practical applications one additional look-up of a log function table, or something equivalent, is negligible in comparison with all other numerical and clerical tasks performed for each collision. But even if this argument does not hold, a correct evaluation of the computer times per collision for AMC and ELP would not change the qualitative picture but only shift the break-even points in the error vs. time curves slightly to the right.

A criticism of the ELP method, based partly on pure reasoning and partly on the detailed analysis of some test runs in respect to the dispersion of neutron weights and to the spatial distribution of collisions in the ELP Monte Carlo game, can be outlined as follows:

(1) A neutron collision occurring quite near to a boundary leads with the high probability of 0.5 to a next collision still nearer to the same boundary.

(2) As a consequence of (1) the rate of collisions in the Monte Carlo game is peaked near the boundary. The average neutron weights associated with collisions in this boundary layer must be low, of course.

(3) For collisions in the boundary layer the normalization factor $A(x,\Omega)$ in Eq. (6) becomes highly dependent on the direction vector Ω, cf. Eq. (5), and may take any value between 0 and 1 with a comparable probability.

(4) From (1) to (3) follows that the dispersion of neutron weights may become very high. In test runs neutrons can be observed at equal times and positions with weights differing by several decades (!).

Method of Controlled Anisotropy in Scattering, CAS

As a consequence of this experience we looked for improvements over ELP by introducing, in addition to track length truncation, angular biassing in the boundary layer with the aim of making long sequencies of collisions in the immediate vicinity of the boundary improbable. The simplest technique to achieve this was named by us the method of Controlled Anisotropy in Scattering (CAS).

Instead of selecting the flight direction Ω from the isotropic distribution, we may introduce at each point x an arbitrary modified angular distribution $F(x,\Omega)$. This can often be done without much additional computing per collision, especially when the distribution is characterized by a few, regionwise constant parameters. When the truncated exponential distribution, Eq. (4), and the new angular distribution $F(x,\Omega)$ are combined, the neutron weight W changes in a scattering collision (at x in direction Ω) from W to

$$W' = W\, A(x,\Omega) \quad 4\pi/F(x,\Omega), \tag{7}$$

with $A(x,\Omega)$ from Eq. (5).

In our spherical test problems we decided to bias only the normal, i.e. radial, component μ of the scattering angle. We choose a fixed value $\mu_1(x)$ with

$$-1 < \mu_1(x) < 1 \tag{8}$$

and put

$$F(x,\mu) = \frac{1}{2(1+\mu_1(x))} \quad \text{for} \quad -1<\mu<\mu_1(x) \tag{9a}$$

$$F(x,\mu) = \frac{1}{2(1-\mu_1(x))} \quad \text{for} \quad \mu_1(x)<\mu<1 \tag{9b}$$

for the probability density of the radial component μ of the flight direction after scattering. Any positive value μ_1 will promote outward scattering, a negative μ_1 promotes inward scattering.

After some experimenting we chose a value of $\mu_1 = -0.3333$ for the outer region of the spheres and $\mu_1 = 0$, corresponding to isotropic scattering, for the inner region. For the larger sphere, Case A, an inner region was defined with a radius $R_i = 2\lambda$ and an outer region between R_i and $R_o = 3\lambda$. For the smaller sphere, Case B, no inner region was defined, i.e. $R_i = 0$.

Also for this version 200 000 collisions have been processed for each case, A and B. That means, that in the comparison with ELP the additional computer time for angular biassing is neglected. This time depends essentially on the type of geometry and is really very small in slab and spherical configurations. Anyhow, a comparison of the estimated errors from ELP and CAS, especially in the Figs. 2, 5, and 6 shows for longer observation times a clear advantage for CAS, which cannot be outweighed by some additional expense in computing.

What seems most important in these results is the proof that the drawbacks inherent in the simple track length truncation method can be overcome to a considerable extent through simple angular biassing schemes. In the test examples shown almost nothing has been done to optimize angular biassing.

Modified ELP method (MELP)

A quite efficient method to control leakage in Monte Carlo has been reported previously (4) under the name of Modified ELP (MELP). It got that name because the numerical realization is very similar to the ELP technique. In the meantime this method turned out to be a special angular biassing scheme combined with track length truncation *. The angular distribution involved in MELP is

$$F(x,\Omega) = \frac{1}{2\pi} \frac{1-\exp(-\Sigma D(x,\Omega))}{2-\exp(-\Sigma D(x,\Omega))-\exp(-\Sigma D(x,-\Omega))} \tag{10}$$

with the previously defined distance function $D(x,\Omega)$.

Note that

$$F(x,\Omega) + F(x,-\Omega) = \frac{1}{2\pi} \tag{11}$$

* I am indebted to Dr. V. Brandl for the clarification of this important question.

For a point far from the boundary $F(x,\Omega)$ of Eq. (10) becomes isotropic as the exponential functions tend to zero. For a point x very near to a boundary the scattering is inward biassed, because then for any outward-directed Ω the distance $D(x,\Omega)$ and the numerator of Eq. (10) become small.

The realization of $F(x,\Omega)$ according to Eq. (10) is surprisingly simple when it is combined with track length truncation. Select Ω from the isotropic distribution, compute $D(x,\Omega)$ and $D(x,-\Omega)$.

$$W_1 = 0.5\ W \exp\ (-\Sigma D(x,\Omega)) \text{ and} \tag{11a}$$

$$W_2 = 0.5\ W \exp\ (-\Sigma D(x,-\Omega)) \tag{11b}$$

are registered as leakage contributions in the time channels corresponding to the leakage times

$$t' = t + D(x,\Omega)/v \qquad (t = \text{collision time}) \text{ and} \tag{12a}$$

$$t'' = t + D(x,-\Omega)/v. \tag{12b}$$

The neutron weight W' after the collision is determined as

$$W' = W - W_1 - W_2 \tag{13}$$

Select a random number ξ from the uniform distribution in the (0,1)-interval and define

$$\xi' = \xi(1-0.5 \exp\ (-\Sigma D(x,\Omega))-0.5 \exp\ (-\Sigma D(x,-\Omega))) \tag{14}$$

If

$$\xi' < 0.5 - 0.5 \exp(-\ \Sigma D(x,\Omega)), \tag{15}$$

then choose Ω as the flight direction and the track length d according to

$$\Sigma d = -\log\ (1 - 2\xi') \tag{16}$$

Otherwise choose $-\Omega$ as the flight direction and the track length d according to

$$\Sigma d = -\log\ (1 - 2\xi'') \text{ with} \tag{17a}$$

$$\xi'' = \xi' + 0.5 \exp\ (-\Sigma D(x,\Omega))-0.5 \tag{17b}$$

This procedure may, in general, be described as follows. From the true, physical, angular distribution a direction Ω is selected and supplemented by a second, equally probable direction Ω'. For isotropic scattering *, that has been assumed for our test problems, we may take

$$\Omega' = -\ \Omega \tag{18}$$

* The more general case of an anisotropic angular distribution is conveniently treated as a transformation of the isotropic distribution.

In both directions the exponential track length distributions are truncated at the associated boundaries. The actual flight direction is finally selected, between Ω and Ω', with probabilities proportional to the associated non-leakage probabilities. This promotes very strongly inward scattering in a boundary area with a width of about one mean free path λ.

With MELP cross section look-up and geometry routines may be invoked twice per collision. A realistic upper limit for the computer time used per collision is, thus, twice the amount for ELP. For this reason with MELP only 100 000 collisions have been processed for each test case and compared with the calculations involving 200 000 collisions for ELP and CAS.

Conclusions

From the comparison of the estimated errors connected with the methods tested we may conclude that in our test problems the collision and leakage rates for long times after the injection of source neutrons are estimated best by a combined scheme of track length truncation and angular biassing in the boundary area. The advantages of such schemes compared to both ELP and AMC are obvious from the figures presented. In the smaller system (Case B, Figs. 5,6) MELP seems superior. In the larger system (Case A, Figs. 2,3) no clear decision in favour of MELP or CAS can be made, as MELP shows lower errors in the leakage estimates, but CAS, which processes more collisions in the same time, yields better estimates of the collision rates.

A possible advantage of a general angular biassing scheme like CAS, over a rather specific scheme like MELP, is that CAS is flexible and depends in a simple fashion on parameters, which can, in principle, even be optimized during the execution of a long-running problem.

Track length truncation, in ELP, CAS, or MELP is used with advantage in those flight directions in which the first and only boundary seen from the collision point is an outer boundary. Otherwise the amount of computation in geometry routines becomes excessive. For neutrons flying in the direction of an inner boundary leakage is more conveniently estimated by the analogue estimator. Especially, all inner regions of an assembly have to be tagged so that after a collision in such a region no track length truncation is performed. But pure angular biassing without track truncation, as a special option of CAS, is possible and useful also in inner regions of an assembly.

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Fig. 5 Error estimates for the collisions per time channel, Case B.

Fig. 6 Error estimates for the leakage per time channel, Case B.

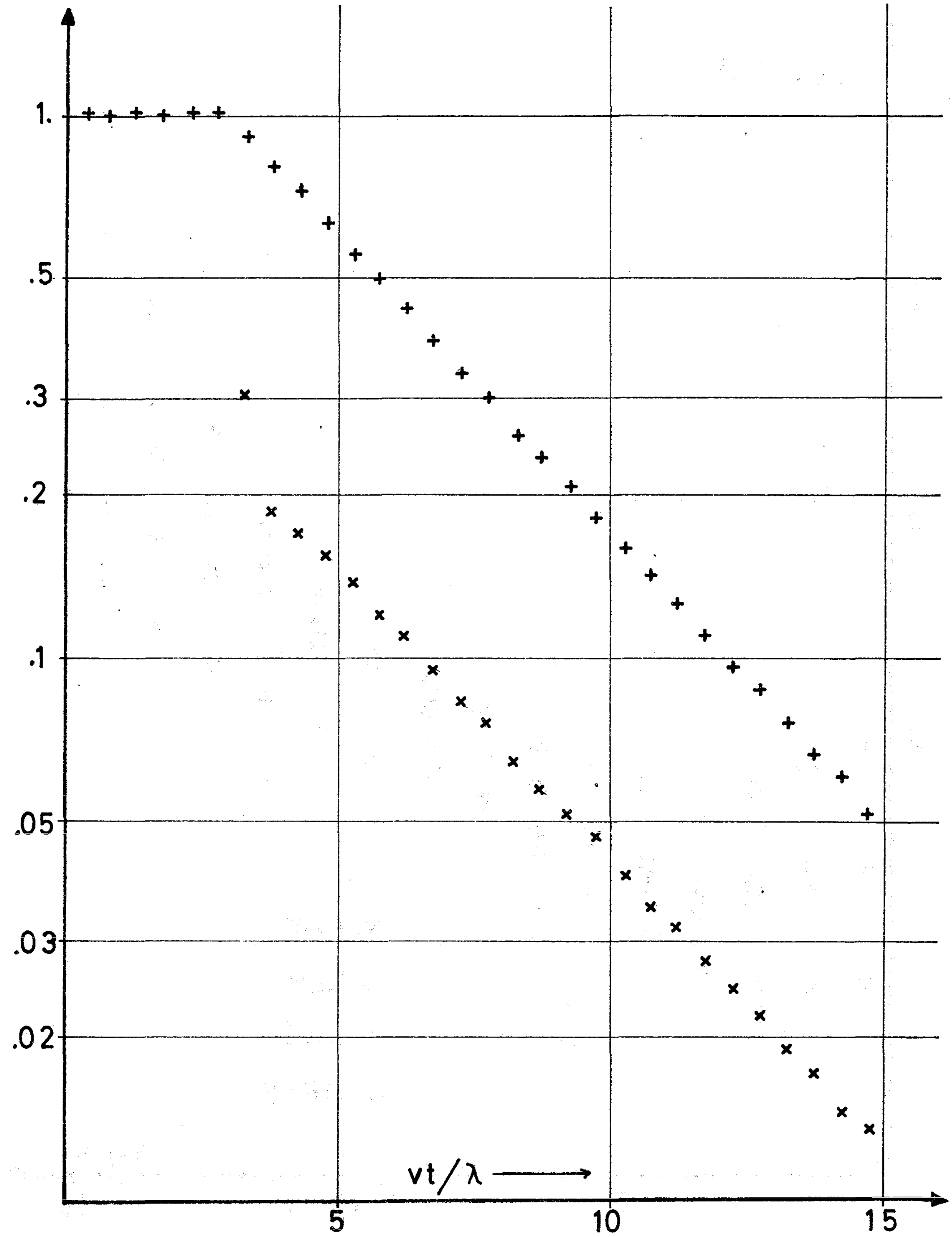

Fig. 1

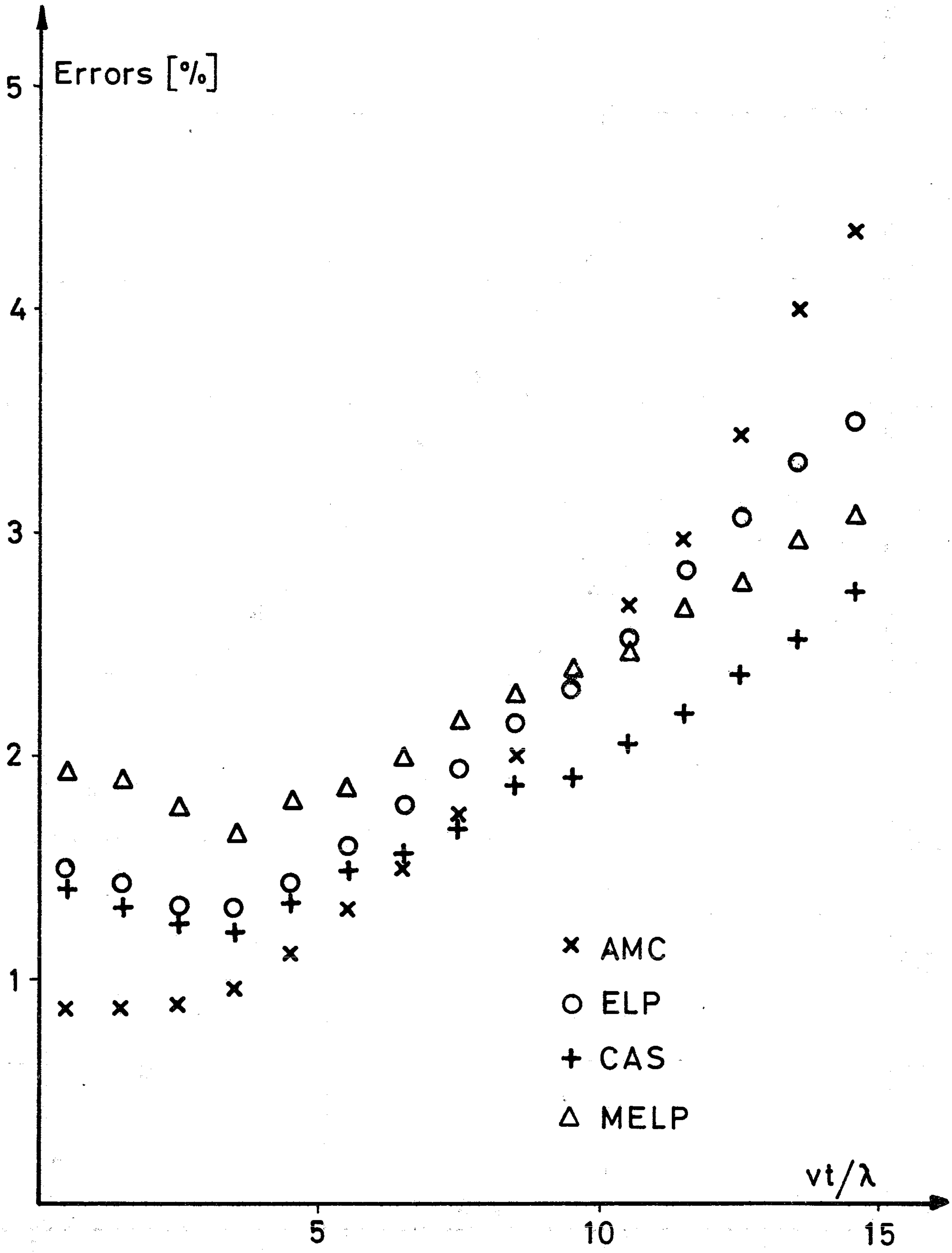

Fig. 2

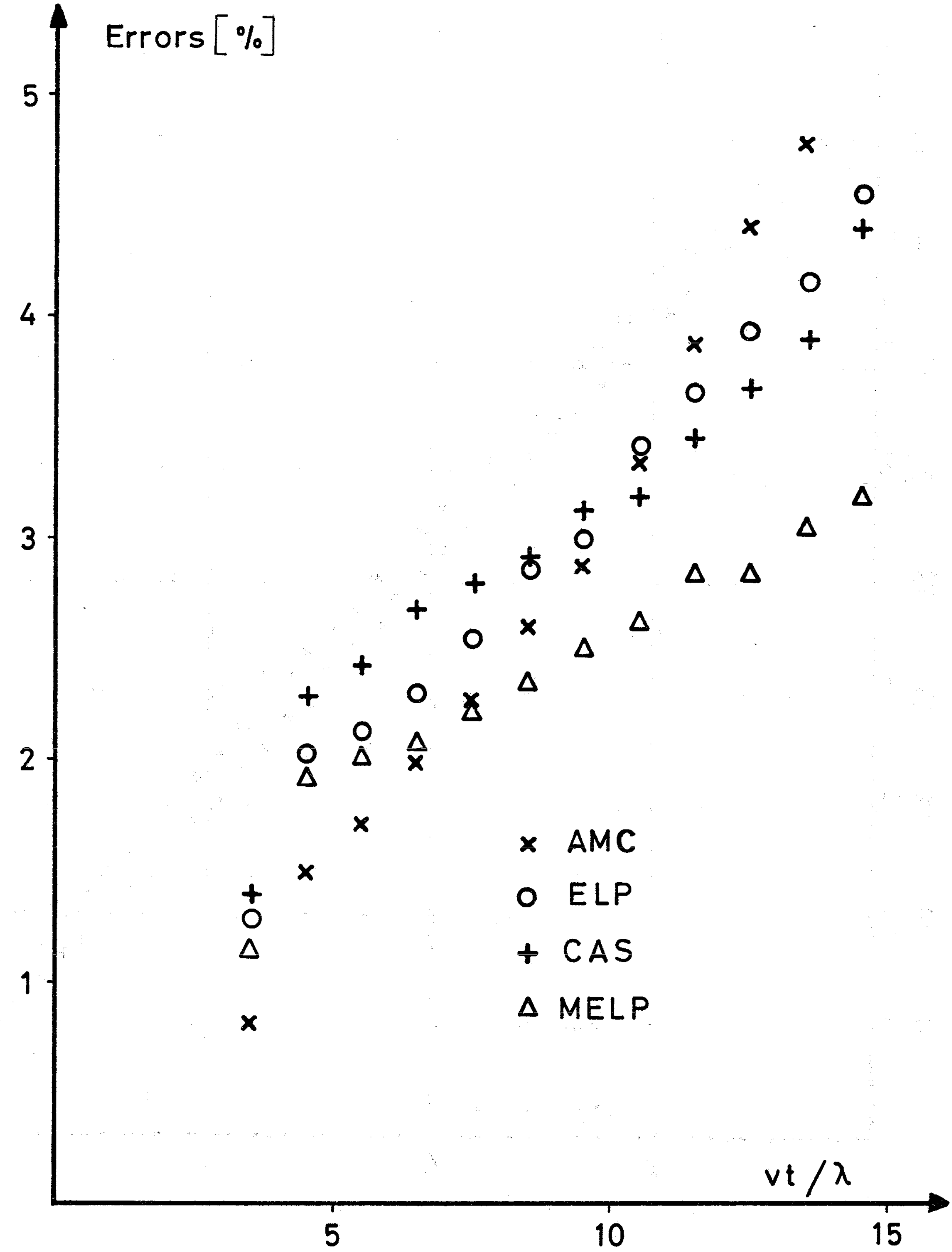

Fig. 3

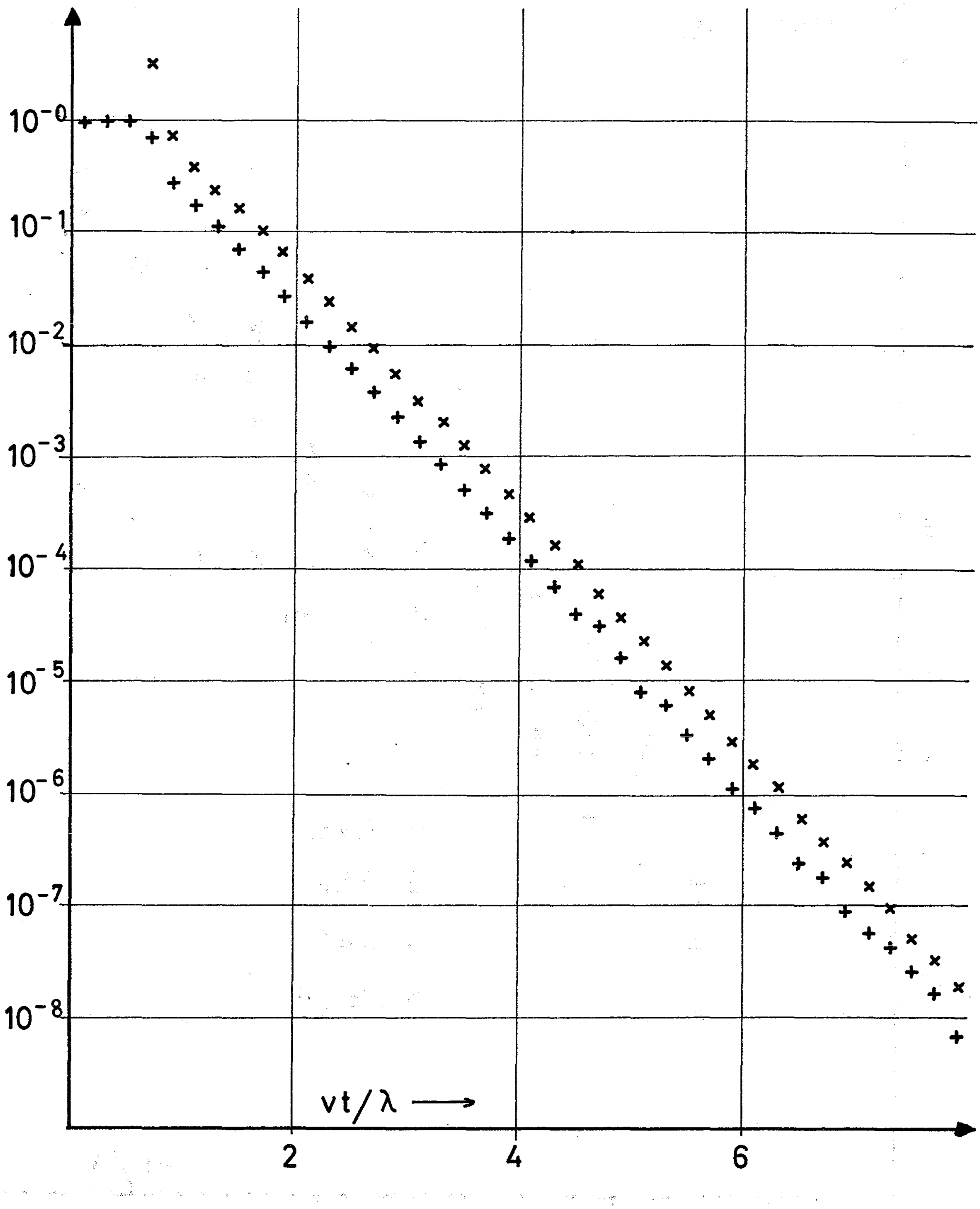

Fig. 4

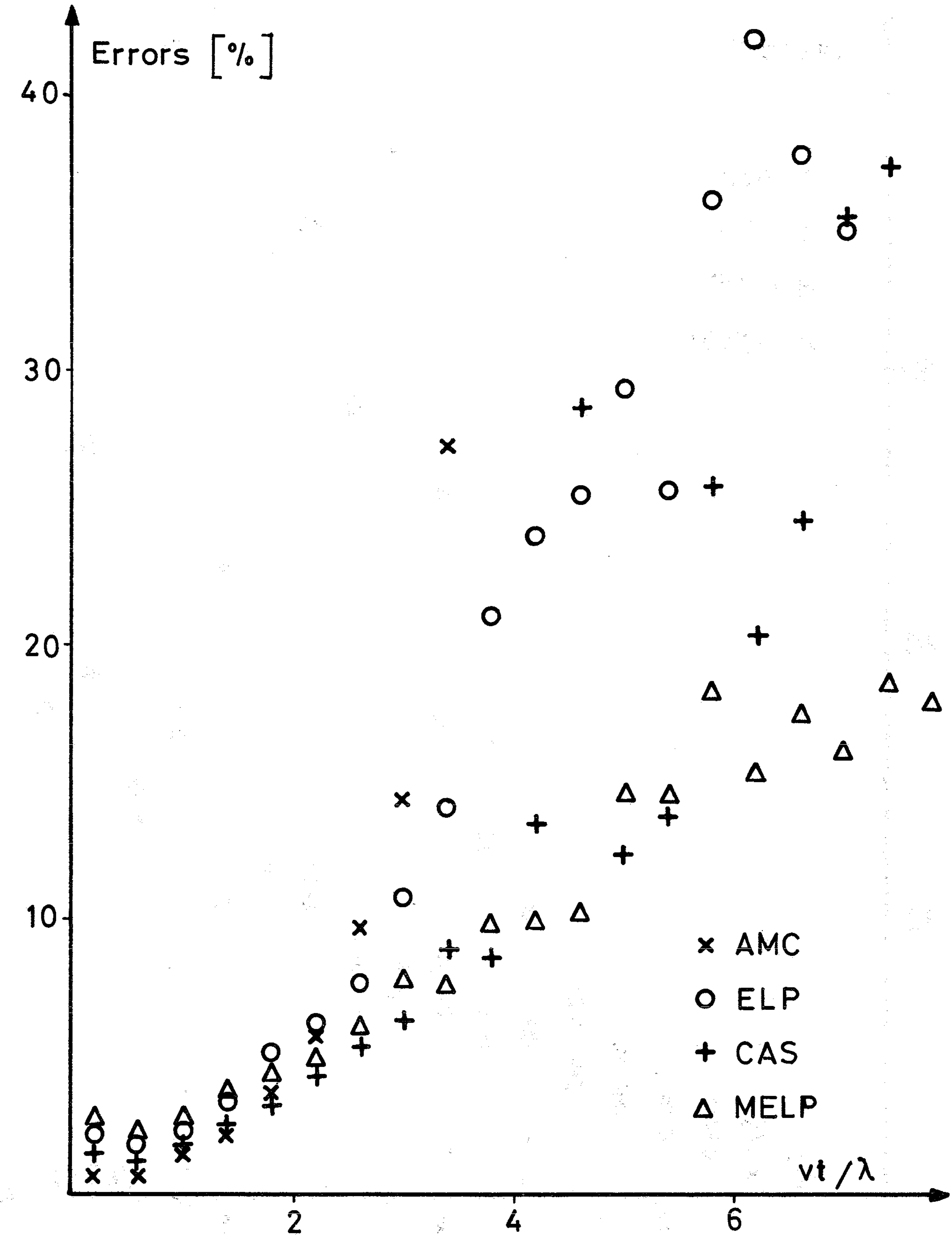

Fig. 5

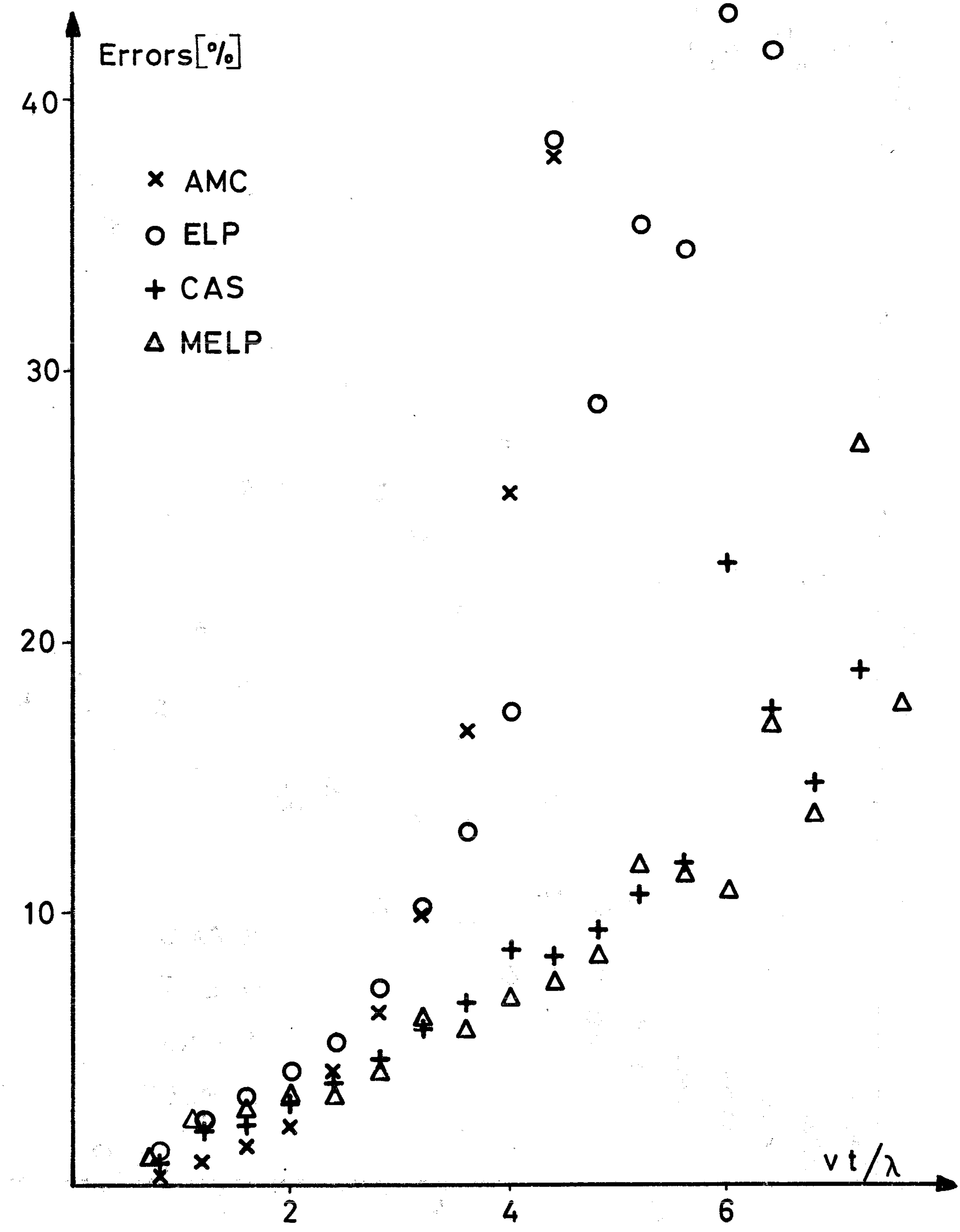

Fig. 6