GENERALIZED QUASISTATIC TRANSPORT SOLUTION OF PROBLEMS WITH EXTERNAL NEUTRON SOURCES

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ABSTRACT

This paper deals with the application of the generalized quasistatic (GQS) approximation to time dependent multigroup transport (and diffusion) equations in hexagonal geometry with high-energy external neutron sources such as those encountered in accelerator-driven systems (ADS). Recent calculations performed on these systems with the classical improved quasistatic (IQS) algorithm due to Ott and Meneley have been far less successful than expected, for reasons that are still rather obscure. One possible explanation lies in the inadequacy of the "amplitude/form" splitting in IQS calculations (with the same amplitude function for all neutron groups) to cope for the physics involved in ADS systems where the neutron energy spectrum ranges from thermal energies to a few tens of MeV. It is surmised that the GQS approximation proposed by Devooght and Mund (with one amplitude function per energy group) is better suited for an accurate treatment of the dynamics of such subcritical systems. We discuss the adaptation of the GQS method to the transport equations in hexagonal geometry in detail.

1. INTRODUCTION

There has been a large interest in recent times in the dynamical behaviour of accelerator driven systems made of a subcritical array of fuel rods sustaining a steady-state fast neutron flux feeded by an external spallation source producing high energy neutrons triggered by accelerated charged particles. The dynamics of such a system, when equilibrium is lost, has its own particular features that must be carefully studied for safety assessment. Several reasons push towards the use of transport theory: ADS systems are rather compact and anisotropy plays an important role in high energy collisions. Among the various numerical methods introduced for the solution of the time-dependent equations, the "quasistatic" family offers a broad spectrum of choices, allowing for computation savings compared with direct integration techniques (see [1]).

The standard quasistatic method used in reactor computations is the improved quasistatic method (IQS) due to Ott and Meneley [2]. In this method the multigroup fluxes are factorized into the product of a time-dependent "amplitude" function (the same for all neutron groups) carrying the greatest part of the time dependence, times a space- *and* time-dependent "form" function (different from group to group) that gives the local changes induced by reactivity variation. Amplitude- and form functions vary on different time scales: a short time-scale related to prompt neutron generation time for the amplitude changes, and a longer time-scale for the form functions, coping for flux tilts. The amplitude function satisfies the point-kinetics equations with coefficients evaluated using the form functions. For their part, the form functions obey a set of time-dependent multigroup equations with source terms due to the amplitude function. In the extreme situation where the space distributions of neutron fluxes is completely insensitive to the reactivity variation, the solution of the time-dependent problem may be obtained at the expense of the sole point kinetics equations.

In this paper we discuss the generalized quasistatic method (GQS) introduced by Devooght and Mund, that considers different amplitude functions depending on the neutron groups. It has been shown earlier that, in traditional chain reacting systems (*i.e.* multiplying systems without "exter-

nal" neutron sources), calculations performed on standard fast- and thermal benchmark problems using the GQS method give results very comparable to those obtained with the IQS algorithm (see for instance the references [3] and [4]). It turns out that this might be different in ADS systems where the neutron population can be subdivided into two different components: spallation neutrons (with a broad energy spectrum) and fission neutrons with their classical energy spectrum. For such systems, IQS calculations have been unsatisfactory in some cases, as reported in the literature [5]. This may be due to the implicit hypothesis that, in the IQS algorithm, all neutrons deliver the same (prompt) dynamical response to a modification of the multiplying properties of the medium. This should not be the case however, for the (high energy) spallation neutrons. The GQS algorithm might therefore help in getting a more comprehensive explanation of such peculiar systems.

Section 2 of the paper summarizes the main features of the GQS algorithm applied to the transport equation in hexagonal-z geometry, i.e. of the HEXNODYN code based on an improved version of Wagner's steady transport method HEXNOD [6] which has been described in [7]; under its original version, HEXNODYN has been described in [8]. In Section 3 we shortly describe the implementation of the GQS algorithm in HEXNODYN. Section 4 discusses the issue of the spallation source more deeply. Finally, Section 5 gives the conclusion.

2. THE GENERALIZED QUASISTATIC FORMALISM

We start with the time-dependent multigroup (with G neutron groups) transport equations with an "external" neutron source, in hexagonal-z geometry:

$$v^{-1}\frac{\partial\overline{\phi}(t)}{\partial t} = A(t)\overline{\phi}(t) + \sum_i \frac{1}{4\pi}\overline{\chi}_i^d\lambda_i C_i(t) + \overline{Q}(t), \qquad \overline{r} \in \mathcal{D}, \quad (1)$$

$$\frac{1}{4\pi}\overline{\chi}_i^d\frac{\partial C_i(t)}{\partial t} = -\frac{1}{4\pi}\overline{\chi}_i^d\lambda_i C_i(t) + J_i^d(t)\overline{\phi}(t), \qquad i = 1,\ldots,I. \quad (2)$$

and suitable boundary- and initial conditions. In these equations $\overline{\phi}(t)$ denotes the vector of angular group fluxes $\phi_g(\overline{r},\overline{\Omega},t)$, $g = 1,\ldots G$ and $\mathcal{D}$ is

the reactor domain. The operator $A(t) = J^p(t) - K(t)$ divides into prompt fission (J^p) and scattering, absorption and transport (K) components, and $v = \mathrm{diag}(v_1, ..., v_G)$. Moreover, $\overline{Q}(t)$ is the G-group external neutron source, C_i the (local) concentration of the i-th family of delayed neutron precursors, $\overline{\chi}_i^{\,d}$ is the i^{th} delayed neutron spectrum and J_i^d the i^{th} delayed neutron production operator with I denoting the total number of delayed-neutrons families. Below, we shall also need the total production operator

$$J \;=\; J^p + \sum_{i=1}^{I} J_i^d \tag{3}$$

For the sake of commodity we deliberately avoid to indicate the space and angular dependence of the fluxes since we are momentarily interested only in the time-dependence of the problem. The equations (1)-(2) form a set of $G + I$ coupled differential equations that can also be written under the following integral form

$$\begin{aligned}
\overline{\phi}(t) \;=\;& \exp(\Omega(t))\,\overline{\phi}(t_0) \\
&+ \int_{t_0}^{t} \exp(\Omega(t) - \Omega(s))\, v \\
&\qquad (A(s) - v^{-1}\,\omega(s) + \sum_i \lambda_i \Gamma_{t,i}(s) J_i^d(s))\overline{\phi}(s) ds \\
&+ \int_{t_0}^{t} \exp(\Omega(t) - \Omega(s))\, v\, \overline{Q}(s) ds \\
&+ \sum_i \frac{\lambda_i}{4\pi} v \overline{\chi}_i^{\,d} \int_{t_0}^{t} \exp(\Omega(t) - \Omega(s) - \lambda_i(s - t_0)) ds\, C_i(t_0)\,, \qquad (4) \\
\frac{1}{4\pi}\overline{\chi}_i^{\,d}\, C_i(t) \;=\;& \frac{1}{4\pi} \exp(-\lambda_i(t - t_0))\overline{\chi}_i^{\,d}\, C_i(t_0) v \\
&\qquad + \int_{t_0}^{t} \exp(-\lambda_i(t - s))\, J_i^d(s)\overline{\phi}(s) ds \qquad (5)
\end{aligned}$$

with

$$\begin{aligned}
\Omega(t) \;&=\; \int_{t_0}^{t} \omega(s) ds\,, \\
\Gamma_{t,i}(s) \;&=\; \int_{s}^{t} \exp(\lambda_i(s - s') + \Omega(s) - \Omega(s')) ds'\,, \qquad (6)
\end{aligned}$$

and where $\omega(t)$ denotes an arbitrary (usually scalar) operator; $A(t)$ and J_i^d are determined from external action including thermohydraulic feedback.

In our approach, these integral equations form the starting point of the quasistatic method. We introduce a splitting of each angular flux $\phi_g(\overline{r}, \overline{\Omega}, t) = T_g(t) \cdot \psi_g(\overline{r}, \overline{\Omega}, t)$ into the product of an amplitude (T_g) and a shape function (ψ_g). The main time-dependence lies in the amplitude, while the time-dependence in ψ_g is entered only to allow modification of flux profiles (the so-called flux "tilts"). One should keep this convention in mind since, as already mentioned, we avoid explicit reference to space- and angular dependence of the unknowns.

In the IQS algorithm of Ott and Meneley, the amplitude functions are the same (T) in all neutron groups. Here however, we assume that it may differ from group to group. The splitting is then conveniently written as one of the following equivalent expressions:

$$\overline{\phi}(t) = \begin{cases} \mathrm{diag}(\psi_g(t)) \cdot \overline{T}(t), & \text{(a)} \\ \\ \mathrm{diag}(T_g(t)) \cdot \overline{\psi}(t), & \text{(b)} \end{cases} \tag{7}$$

where in both cases the elements along the matrix diagonal (ψ_g or T_g, $1 \leq g \leq G$) are different from each other. To ensure unicity of the "amplitude $\times$ shape" splitting, the following condition applies to all groups at any time:

$$< \phi_g^\star, \frac{1}{v_g}\, \psi_g(t) >= 1, \qquad \forall\, t \geq 0, \qquad 1 \leq g \leq G, \tag{8}$$

where $\phi_g^\star$ is a time-independent spatio-angular weighting function and the bracket notation $< u, v >$ indicates the inner product of u and v:

$$< u, v >= \int_{4\pi} d\overline{\Omega} \int_{\mathcal{D}} d\overline{r}\, u(\overline{r}, \overline{\Omega}) \cdot v(\overline{r}, \overline{\Omega}). \tag{9}$$

In this integral, $\mathcal{D}$ denotes the domain of the problem.

Let Ψ denote the diagonal matrix in the splitting (7.a). We introduce this expression into (4), multiply to the left by the diagonal matrix of weighting functions $\Phi^* = \mathrm{diag}(\phi_g^\star)$ and perform the inner product (9). Taking the splitting constraint (8) into account, we get

$$\begin{aligned} \overline{T}(t) &= \exp(\Omega(t))\, \overline{T}(0) \\ &+ \int_{t_0}^{t} \exp(\Omega(t-s)) \end{aligned}$$

$$\left(F\rho(s) - F\beta(s) + \sum_i \lambda_i \Gamma_{t,i}(s) F\beta_i(s) - \omega(s) F\Lambda(s) \right) \overline{T}(s) ds$$

$$+ \int_{t_0}^{t} \exp(\Omega(t-s)) \overline{q}(s) ds$$

$$+ \sum_i \lambda_i \int_{t_0}^{t} \exp\left(\Omega(t) - \Omega(s) - \lambda_i(s-t_0)\right) ds\, \overline{\eta}_i(t_0), \tag{10}$$

$$\overline{\eta}_i(t) = \exp(-\lambda_i(t-t_0)) \overline{\eta}_i(t_0) + \int_{t_0}^{t} \exp(-\lambda_i(t-s)) F\beta_i(s) \overline{T}(s) ds, \quad 1 \le i \le I, \tag{11}$$

with the following notation

$$\begin{aligned}
F\Lambda(t) &= \int_{4\pi} d\overline{\Omega} \int_{\mathcal{D}} d\overline{r}\, \Phi^* v^{-1} \Psi(t) = I \\
F\rho(t) &= \int_{4\pi} d\overline{\Omega} \int_{\mathcal{D}} d\overline{r}\, \Phi^* (J(t) - K(t)) \Psi(t), \\
F\beta_i(t) &= \int_{4\pi} d\overline{\Omega} \int_{\mathcal{D}} d\overline{r}\, \Phi^* J_i^d(t) \Psi(t), \\
F\beta(t) &= \sum_i F\beta_i(t), \\
\overline{\eta}_i(t) &= \int_{4\pi} d\overline{\Omega} \int_{\mathcal{D}} d\overline{r}\, \Phi^* \frac{1}{4\pi} \overline{\chi}\, C_i(t), \\
\overline{q}(t) &= \int_{4\pi} d\overline{\Omega} \int_{\mathcal{D}} d\overline{r}\, \Phi^* \overline{Q}(t).
\end{aligned} \tag{12}$$

Note that $F\Lambda$, $F\rho$, $F\beta_i$ and $F\beta$ are all $G \times G$ matrices. The equations (10)-(12) generalize the $(G+I)$ multigroup point kinetics (MPK) equations in integral formulation. The solution to these equations depends on the evaluation of the various matrix and vector quantities defined by (12) which essentially rests on the knowledge of the multigroup shape functions $\psi_g(\overline{r}, \overline{\Omega}, t)$.

Introducing the splitting (7.b) into (4) one gets an equation that can be viewed as the reference equation for the shape functions $\psi_g(\overline{r}, \overline{\Omega}, t)$. But then, one must assume some (approximate) knowledge of the amplitudes functions $T_g(t)$. Clearly the determination of $T_g(t)$ and $\psi_g(t)$ has to be performed iteratively.

The time discretization of the quasistatic equations uses two time scales: a micro-time step h for $T_g(t)$ and a macro-time step $H = nh$ for $\psi_g(t)$. Assume amplitudes and shapes have been determined at the end of some macro-time

step corresponding to $t_\star$. The GQS algorithm in the next macro-time step $[t_\star, t_\star + H]$ goes then as follows:

- Setting $\psi_g^{(0)}(t_\star + H) = \psi_g(t_\star)$, evaluate the MPK matrix operators ($F\rho^{(0)}$, $F\beta_i^{(0)}$, $F\beta^{(0)}$) at $t = t_\star + H$ using (12) as a first guess and interpolate these parameters on the micro-time step $t_\star + kh$, with $1 \leq k \leq (n-1)$,
- Solve the MPK equations (10) giving $T_g^{(0)}(t_\star + kh)$ on the micro-time scale, up to $t_\star + H$,
- Solve the shape equations (i.e. Eq. (4) with the splitting (7.b), under the constraint that $F\Lambda(t_\star + H) = I$), assuming the current value of the amplitudes $T_g^{(0)}(t_\star + H)$, in order to get $\psi_g^{(1)}(t_\star + H)$. This is followed by a new evaluation of the MPK matrix operators ($F\rho^{(1)}$, $F\beta_i^{(1)}$, $F\beta^{(1)}$),
- Iterate this process, up to convergence and proceed to the next macro-time step.

To complete this summary of the GQS algorithm, we have still to indicate how the quadratures appearing in (10) and in (4)-(7.b)) are evaluated in practice. This is usually done replacing the integrand by a suitable interpolation formula. For instance, on a micro-time step $[kh, (k+1)h]$, $k = 0, ..., (n-1)$, the amplitude $T_g(t)$ in the g-th neutron group is approximated by:

$$T_g(t) \;\approx\; T_g(kh)\,\theta_{k,1}(t) \;+\; T_g((k+1)h)\,\theta_{k,2}(t), \tag{13}$$

where the interpolation functions $\theta_{k,j}$ satisfy the (cardinality) conditions:

$$\begin{array}{ll} \theta_{k,1}(kh) = 1, & \theta_{k,1}((k+1)h) = 0, \\ \theta_{k,2}(kh) = 0, & \theta_{k,2}((k+1)h) = 1. \end{array} \tag{14}$$

Similar expansions are used on the macro-time scale (see below § 3). Linear functions correspond here to the well-known Crank-Nicolson scheme. More sophisticated schemes can be used as well that allow, for instance, for spectral matching (see, for instance [9]).

We emphasize again that the main difference between the IQS and GQS algorithm lies in the fact that the latter allows for more flexibility in the

amplitude-shape splitting with one amplitude per neutron group. Another difference lies in the choice of the time integration basis functions $\theta_{k,j}$ where in the IQS case the choice is very specific: Volodka's method (a variant of the Padé's P_{22} algorithm) for the pointkinetics equations and the implicit Euler algorithm for the shapes.

3. GQS IMPLEMENTATION IN HEXNODYN

In HEXNODYN, an operator $B(t)$ acting on the function $\overline{\phi}(t) = T(t)\overline{\psi}(t)$ is represented on a macro-time step $[0, H]$ by:

$$\begin{aligned} B(t)\overline{\phi}(t) &= B(t)T(t)\overline{\psi}(t) \\ &\approx (B(0)T(t)\overline{\psi}(0))\,\varphi_1^\star(t) + (B(H)T(t)\overline{\psi}(H))\,\varphi_2^\star(t) \end{aligned} \tag{15}$$

with interpolation basis functions satisfying

$$\begin{array}{ll} \varphi_1^*(0) = 1 & \varphi_1^*(H) = 0 \\ \varphi_2^*(0) = 0 & \varphi_2^*(H) = 1 \end{array} \tag{16}$$

The same technique can be kept here with $T(t)$ now understood as the diagonal matrix $T(t) = \mathrm{diag}(T_g(t))$. It might also be advisable to use distinct basis functions for flux interpolation and for source interpolation since there is no need to achieve spectral matching for $q(t)$.

The shape equations are obtained in this way, by inserting the interpolation quadrature scheme (15) into (4), giving on the current macro time step $[0, H]$,

$$K(H)\overline{\psi}(H) = \tilde{J}(H)\overline{\psi}(H) + v^{-1}\overline{S} \tag{17}$$

to be solved under the constraint

$$F\Lambda(H) = \int_{4\pi} d\overline{\Omega} \int_{\mathcal{D}} d\overline{r}\, \Phi^* v^{-1} \Psi(H) = I\,. \tag{18}$$

Here

$$\tilde{J}(H) = J^p(H) + \sum_i \lambda_i f_{i2} g_2^{-1} J_i^d(H) - v^{-1}(\omega(H) + g_2^{-1}T(H)) \tag{19}$$

and

$$
\begin{aligned}
v^{-1} g_2 \overline{S} \;=\; & \sum_i \lambda_i h_i \frac{1}{4\pi} \overline{\chi}_i^d C_i(0) + \hat{g}_1 \overline{Q}(0) + \hat{g}_2 \overline{Q}(H) \\
& + v^{-1} (\exp(\Omega(H)) T(0) - \omega(0) g_1) \overline{\psi}(0) \\
& + g_1 (J^p(0) - K(0)) \overline{\psi}(0) + \sum_i \lambda_i f_{i1} J_i^d(0) \overline{\psi}(0), \qquad (20)
\end{aligned}
$$

where

$$
\begin{aligned}
f_{ij} &= \int_0^H \exp(\Omega(H) - \Omega(t)) \Gamma_{H,i}(t) T(t) \varphi_j^*(t) dt \,, \\
g_j &= \int_0^H \exp(\Omega(H) - \Omega(t)) \varphi_j^*(t)\, T(t) dt \,, \\
\hat{g}_j &= \int_0^H \exp(\Omega(H) - \Omega(t)) \varphi_j^*(t) dt \,, \\
h_i &= \int_0^H \exp(\Omega(H) - \Omega(t) - \lambda_i t) dt \,,
\end{aligned} \qquad (21)
$$

with $i = 1, \ldots, I$ and $j = 1, 2$. Note that f_{ij} and g_j are now $G \times G$ matrices since $T(t)$ is a $G \times G$ matrix.

It should further be noticed here that the equations (17) and (18) are compatible since this requirement is equivalent to the existence of a generalised quasistatic solution. Together they represent after discretization with say N discrete unknowns per group, a rank deficient linear system, of order $NG + G$ but of rank NG and this system is compatible, i.e. it has a unique solution.

To appropriately generalize the solution procedure implemented in HEXNODYN we first rewrite (17) under the form

$$
K_{pr} \overline{\psi}(H) = (\tilde{J}(H) - \Delta K_{pr}) \overline{\psi}(H) + v^{-1} \overline{S} \qquad (22)
$$

where K_{pr} is an approximation of $K(H)$ and $\Delta K_{pr} = K(H) - K_{pr}$. This must be solved under the constraint (18) which may be rewritten

$$
< \phi_g^*, (1/v_g)\, \psi_g(H) >= 1 \quad g = 1 \ldots G \,, \qquad (23)
$$

and means that the orthogonal projection of each component $\psi_g(H)$ of $\overline{\psi}(H)$ onto the corresponding component $(1/v_g)\, \phi_g^*$ of $v^{-1} \overline{\phi}^*$ must be unity.

Because the shape equations and the constraint are compatible, there is no loss of generality in projecting the $\psi_g(H)$ equation onto $((1/v_g)\, \phi_g^*)^\perp$,

the orthogonal complement of $(1/v_g)\,\phi_g^*$. The projector P on $((1/v_g)\,\phi_g^*)^\perp$, parallel to $\psi_g(H)$ is

$$u_g \rightarrow Pu_g = u_g - \frac{< \phi_g^*, (1/v_g)\,u_g >}{< \phi_g^*, (1/v_g)\,\psi_g(H) >}\psi_g(H) \tag{24}$$

or

$$u_g \rightarrow Pu_g = u_g - < \phi_g^*, (1/v_g)\,u_g > \psi_g(H) \tag{25}$$

because of the constraint (23). Therefore, writing(22) under the form

$$\psi_g(H) = [K_{pr}^{-1}((\tilde{J}(H) - \Delta K_{pr})\overline{\psi}(H) + v^{-1}\overline{S})]_g \tag{26}$$

and projecting both members on $((1/v_g)\,\phi_g^*)^\perp$, parallel to $\psi_g(H)$ gives

$$0 = [K_{pr}^{-1}((\tilde{J}(H) - \Delta K_{pr})\overline{\psi}(H) + v^{-1}\overline{S})]_g - \alpha_{gg}\psi_g(H) \tag{27}$$

i.e.

$$\alpha_{gg}\psi_g(H) = [K_{pr}^{-1}((\tilde{J}(H) - \Delta K_{pr})\overline{\psi}(H) + v^{-1}\overline{S})]_g \tag{28}$$

with

$$\alpha_{gg} =< \phi_g^*, (1/v_g)\,[K_{pr}^{-1}((\tilde{J}(H) - \Delta K_{pr})\overline{\psi}(H) > + v^{-1}\overline{S})]_g \tag{29}$$

This may be written under the form

$$K_{pr}\alpha\overline{\psi}(H) = (\tilde{J}(H) - \Delta K_{pr})\overline{\psi}(H) + v^{-1}\overline{S} \tag{30}$$

with $\alpha = \mathrm{diag}(\alpha_{gg})$ and solved by the iteration scheme

$$\overline{\psi}_{s+1}(H) = \alpha_s^{-1}K_{pr}^{-1}(\ (\tilde{J}(H) - \Delta K_{pr})\overline{\psi}_s(H) + v^{-1}\overline{S}\ ) \tag{31}$$

with $\alpha_s = \mathrm{diag}(\alpha_{gg}^{(s)})$ computed from

$$\alpha_{gg}^{(s)} =< \phi_g^\star, (1/v_g)\,[K_{pr}^{-1}((\tilde{J}(H) - \Delta K_{pr})\overline{\psi}_s(H) + v^{-1}\overline{S})]_g > \tag{32}$$

4. DISCUSSION

The IQS method attempts to split the flux variation into a rapidly changing amplitude and a slowly varying shape depending on all variables but hopefully moderately depending on time. The amplitude evolution is governed

by the point kinetics equations and, in successful cases, the shape equation needs be solved only a few times, the transient being mainly driven by the point kinetics. The GQS method is similar but it leads to a rather unusual version of point kinetics which we have written in our developments under its integral form since this is better suited to numerical handling. Its differential form may be written

$$\frac{d\overline{T}(t)}{dt} = (F\rho(t) - F\beta(t))\overline{T}(t) + \sum_i \lambda_i \overline{\eta}_i(t) + \overline{q}(t) \quad (33)$$

$$\frac{d\overline{\eta}_i(t)}{dt} = -\lambda_i \overline{\eta}_i(t) + F\beta_i(t)\overline{T}(t) \quad (34)$$

and we recall that the point kinetics parameters $F\rho(t)$, $F\beta_i(t)$ and $F\beta(t)$ now appear as $G \times G$ matrices. These equations have not yet been analysed separately and this should be the first gap to fill in further developments of the GQS method since in the best suited cases, one could rest on their sole solution. Their advantage with respect to the usual point kinetics equations is to care for spectral variations. Actually, "shape function" is a somewhat misleading term in the IQS method because angle and energy are also shape variables. This entails in particular that rapid spectral variations cannot be properly handled by the IQS method. Such rapid spectral variations are however expected to happen in ADS transients and this is the basic motivation of our proposed approach.

Another important issue to take care of is the anisotropy of both the source and the scattering at high energy. The method implemented in HEXNOD [7] can be generalised to handle both aspects but with quite different workload requirements. The inclusion of anisotropic sources represents only a moderate work but the adaptation to anisotropic scattering will require heavy technical developments.

5. CONCLUSION

In this contribution, we have proposed a practical application of the GQS formalism introduced by Devooght and Mund in [3] and prepared the steps needed for its implementation in the 3D kinetic transport code HEXNODYN.

Numerical results are not yet available at this stage and we would have delayed the present work until completion of the code adaptations under normal circumstances, but we thought necessary to make this preliminary contribution now to honor the memory of our teacher Jacques Devooght.

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