State University of New York Report

Large Eddy Simulations and Direct Numerical Simulations of High Speed Turbulent Reacting Flows

by

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Semi-Annual Report Submitted to
NASA Langley Research Center

Summary of Activities Supported Under Grant NAG 1-1122

for the Period

May 1, 1991 - October 31, 1991

Contents

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Abstract

This main objective of this research is to extend the boundaries within which *Large Eddy Simulations* (LES) and *Direct Numerical Simulations* (DNS) can be applied in computational analyses of high speed reacting flows. In the efforts related to LES, we have been concerned with developing reliable subgrid closures for modeling of the fluctuation correlations of *scalar* quantities in reacting turbulent flows. In the work on DNS, we have focused our attention to further investigate the effects of exothermicity in compressible turbulent flows. In our previous work, in the first year of this research, we have considered only "simple" flows. Currently, we are in the process of extending our analyses for the purpose of modeling more practical flows of current interest at NASA Langley Research Center.

This report provides a summary of our accomplishments during the third six months of the research supported under Grant NAG 1-1122 sponsored by NASA Langley Research Center administrated by Dr. J. Phil Drummond of the Theoretical Flow Physics Branch.

1 Introduction

During the second year of activities under this research, we have been primarily involved with the continuations of our tasks in the same two directions as those followed in the first year. Namely: (1) development of subgrid closures for LES of compressible reacting flows, and (2) understanding the mechanisms of mixing and reaction in high speed combustion. In the efforts related to the first task, we have undertaken the simulations of homogeneous reacting turbulence, whereas in the second task, DNS of a reacting planar jet is the subject of main focus. Below, a summary of our efforts during the first 6 months of this research in the second year is provided and detail descriptions are furnished in Appendix I and Appendix II.

1.1 Large Eddy Simulations of Compressible Reacting Flows

Our major goal in this effort is to initiate a program to extend the present capabilities of LES for the treatment of chemically reacting flows. In the efforts to date, we have been primarily concerned with *a priori* analysis of subgrid fluctuation in a compressible homogeneous flows. This analysis is mainly involved with constructing the shapes of the simulated Probability Density Functions (PDF's) within the subgrid. Based on our efforts thus far, we have been able to demonstrate that in the context of single-point PDF formulation, the mapping closure of Kraichnan [1] provides the most satisfactory results. The main deficiency of this mapping closure (or any other single-point PDF model) is associated with its incapability in predicting the frequency (or length) scale of PDF evolution. At this stage, unfortunately, the extension of the mapping closure for PDF formulation at two-point is very difficult. Among the currently available alternatives, the EDQNM spectral closure [2] provides a reasonable remedy to overcom this deficiency, but at the present stage cannot be yet implemented for the modeling of compressible turbulent flows.

With the utilization of the mapping closure, the limiting rate of fuel consumption in homogeneous flows can be predicted by a closed form mathematical relation. The results obtained by this relation compares very well with DNS data. In the firs year, our

results were valid only for *stoichiometric* mixtures. In the second year, we have extended our analysis for the modeling of non-unity equivalence ratio mixtures. To the best of our knowledge, this relation is more satisfactory than any other suggested correlations (empirical or theoretical) available in the literature within the past thirty years!

In addition to these conclusions, we have also been able to demonstrate that the β-density [3] does reasonably well in approximating the single point PDF distribution of a conserved scalar property, if the evolution of its variance is known *a priori*. With the implementation of this density, it is also possible to develop a closed form algebraic solution for the limiting rate of reactant conversion under all equivalence ratios. However, despite its simplicity the β-density is only applicable for description of "simple" distributions. It is not applicable for trimodal distributions, and it can not predict the subsequent evolution of the PDF, if the distribution is not of β-type initially. Furthermore, it can not be extended for predictions of non-equilibrium reactions and there are no firm mathematical proofs to justify its use.

At this stage, we have not yet applied the mapping closure for the modeling of practical flows. However, the model based on the β-density has proven somewhat useful for the purpose of *turbulence modeling* in free shear flows. Appendix I provides a summary of our activities in this regard. The extension of our work for the purpose of *subgrid closures* in such flows, is the subject of our current investigation.

1.2 Direct Numerical Simulations of an Exothermic Reacting Planar Jet

Our efforts in this work have been focused on elucidating the role of exothermicity in an unpremixed reacting planar jet flame. This work has been mainly motivated due to the interest of NASA in understanding the global and detail mechanisms of mixing and chemical reactions in high speed jet flames.

In this work, results are obtained of DNS of a compressible, spatially developing, forced planar jet under the influence of a finite rate chemical reaction of the type $F + O \rightarrow$ Product + Heat. Our results suggest that in the setting of a "turbulent" flame, the effect of the heat liberated by the chemical reaction is to *increase* the rate of reactant

conversion. This finding is different from the conclusions of earlier DNS results and laboratory investigations which indicate a suppressed chemical reaction with increasing heat release. However, this conclusion is established only in the context of the simplified kinetics mechanism adopted here, and its extent of applicability for practical flames requires laboratory measurements.

We are presently at a preliminary stage of our work on this issue. A summary of our findings to date is provided in Appendix II.

2 Publications and Honors

The following publications have resulted from our efforts during the first phase of the second year of this research:

1. S.H. Frankel, C.K. Madnia, and P. Givi, "Modeling of the Reactant Conversion Rate in a Turbulent Shear Flow," *Chem. Eng. Comm.*, in press (1992).

2. C.J. Steinberger, "Model Free Simulations of a High Speed Reacting Mixing Layer", AIAA Paper *92-0257* (1992).

Mr. Craig Steinberger was invited to participate at the AIAA 30th Aerospace Sciences Meeting, held in Reno, Nevada, to present his AIAA paper listed above.

3 Appendix I

This appendix has been prepared by Mr. Steven Frankel and Dr. Cyrus Madnia. Dr. Madnia is currently being partially supported by this grant.

Problem Description

The problem under consideration is that of a spatially evolving mixing layer containing initially segregated reactants A and B in the two free streams. Species A is introduced into the upper, high-speed stream and species B enters on the lower, low-speed side. The chemical reaction between the two species is assumed to be single step, irreversible and infinitely fast. The magnitude of the Mach number is assumed negligible. Therefore, the flow is considered incompressible. The two species are assumed thermodynamically similar with identical diffusion coefficients. Within the framework of these approximations, the flow is mathematically described by the conservation equations of mass, momentum, and a species conservation equation for the trace of a conserved Shvab-Zeldovich variable $\mathcal{J}$, which characterizes the compositional structure of the flow. These equations are parameterized by the Reynolds number, the Peclet number, and the velocity ratio across the layer.

The computational package employed in the DNS is based on a hybrid pseudospectral-spectral element algorithm developed in [4, 5]. The pseudospectral routine, which is based on Fourier collocation, is used in the cross stream direction together with free slip boundary conditions. The spectral-element discretization is employed in the streamwise direction. This involves the decomposition of the domain in this direction into an ensemble of macro finite elements. Within each of these elements, the dependent flow variables are approximated spectrally by means of Tchebysheff polynomials of the first kind. The hybrid procedure employed in this way is very attractive in that it combines the accuracy of spectral discretization with the versatility of finite element methods. Therefore, it is convenient for accurate simulations of the complex spatially developing flow under consideration here. For a detailed description of this hybrid method for DNS

of turbulent shear flows, the reader is referred to [5].

The flow field is initialized at the inflow by a hyperbolic tangent mean velocity distribution, upon which low amplitude perturbations are superimposed in order to promote the formation of coherent vortices. The initialization of the Shvab-Zeldovich parameter at the inflow is such that it takes on the values of zero and one in the streams containing B and A, respectively. The disturbances on the mean flow correspond to the most unstable mode of the hyperbolic tangent profile [6] and its first two subharmonics. The amplitude of the fluctuating velocity is set equal to 6% of the mean velocity. This amplitude corresponds to that measured in typical shear layer experiments. The magnitudes of the phase shifts between the modes of the instability waves are randomly selected from a random seed with a top hat PDF of zero mean and a specified variance. The implementation of these phase shifts is the only mechanism to introduce randomness into an otherwise deterministic simulation. This is to partially mimic the random "commotions" which are present in the "universe," into an isolated two-dimensional simulation. At the outflow, a weak condition of zero second derivative is applied for all the dependent variables. This boundary condition cannot be justified in a rigorous mathematical sense and can be specified only in an *ad hoc* manner. This was done in order to facilitate implementation of the Dirichlet boundary conditions in the finite element procedure employed here. Moreover, the results of extensive numerical tests showed that the effects of the approximate boundary condition are confined to within the last computational element. This is consistent with that found previously in [7]. Therefore, the solution in the last computational domain can be ignored.

With the solution of the unsteady transport equations, the DNS data are extremely useful in visualizing the instantaneous behavior of the flow. The results of these direct simulations can also provide an assessment of the statistical behavior of the flow. This is due to the availability of flow information at all the computational grid points and at all times. Therefore, statistical sampling can be done quite easily by ensemble averaging of the instantaneous data gathered over many realizations.

In our simulations the instantaneous data of the Shvab-Zeldovich variable, obtained from the DNS, are used for statistical analysis. A total of 3200 realizations were employed in the sampling. With this ensemble, the magnitudes of the mean and the variance of the

Shvab-Zeldovich variable are calculated at all the grid points. These statistical quantities are of primary interest for turbulence modeling. Based on the knowledge of these first two moments, a Beta density is assumed for the PDF of the Shvab-Zeldovich variable. The ensemble mean values of the product concentration and the unmixedness are calculated subsequently via this density. These modeled quantities are then compared with those obtained directly from the DNS data. Due to the spatial inhomogeneity of the flow the mixture is not stoichiometric at all the grid points. Therefore, the Beta density is usually asymmetric at majority of these points.

Presentation of Results

Computations were performed in a domain of size $13\delta \times 34\delta$, where δ denotes the vorticity thickness at the inlet of the flow. There are 65 Fourier modes in the cross-stream direction and 42 finite elements are used for the streamwise discretization. A fifth order Tchebysheff polynomial is employed to approximate the variables within each element. This discretization is equivalent to, at least, a fifth order accurate finite difference technique even if the spectral convergence is not considered. This results in a total number of 211 points in the streamwise direction. A second-order Adams-Bashforth finite difference scheme was utilized for temporal discretization. With the computationally affordable 211×65 grid resolution available, accurate simulations with $Re = Pe = 200$ (where these normalized quantities are defined based on the velocity difference across the layer, and the initial vorticity thickness) are possible [8]. These values are somewhat smaller than those of a fully developed laboratory turbulent shear layer, but are sufficiently high to promote the growth of instability waves.

In order to visualize the flow evolution, a time series of DNS generated snapshots of the instantaneous normalized product concentration are shown in Fig. 1. This figure depicts the way in which the small amplitude perturbations manifest themselves in the formation of large scale coherent vortices downstream of the splitter plate. The forcing associated with the most unstable mode alone would cause the initial roll-up of these vortices. The perturbations corresponding to the first subharmonic mode result in a second roll-up in

the form of merging neighboring vortices, and the presence of the second subharmonic generates a third roll-up (second merging) at a region near the outflow. The roll-up and the subsequent pairings of these vortical structures engulf the unreacted species from the two streams into the mixing zone. The dynamics of the vortical evolution in this process reflect the two main mechanisms of mixing enhancement. Large concentrations of vorticity, that are approximately of one sign, bring the fluid from the two free streams into the large scale structures. Within these structures, the fluid elements are subject to further straining, and diffusion between the two fluids results in final mixing at the molecular scale. With these processes, along with the assumption of infinitely fast chemistry, the rate of product formation is naturally enhanced by the dynamics of vortical evolution.

To demonstrate the capability of the model based on the Beta density, the cross stream variation of the product concentration and those of the negative of the unmixedness are presented at two streamwise locations in Figs. 2-3. Also the streamwise variation of the total product, T_p, is presented in Fig. 4. In all these figures, the comparisons between the model predictions and the DNS results are noteworthy. The agreements demonstrated by these comparisons provide a reasonable justification for recommending Beta density as working relations in routine engineering predictions. However, these relations are advocated only for statisticanl predictions of low order moments. The physics of the mixing phenomenon in a spatially developing shear flow is far too complex to be *completely* described by the Beta density. The highly intermittent nature of the mixing process exhibits features that cannot be fully captured by this density [8]. To demonstrate this point quantitatively, in Figs. 5-6 the cross stream variations of the third and fourth centralized moments of the Shvab Zeldovich variable calculated from the β density are compared with those generated by DNS. These figures indicate that while the trend is somewhat similar in the two cases, the extent of agreement is not as good as those of lower level statistical quantities (Figs. 2-4). This is primarily due to the mechanism of large scale entrainment in the shear flow, in that there are always unmixed fluids present within the core of the vortical structures. This results in a slight trimodal behavior in the probability distributions generated by DNS and observed experimentally [4, 9, 10, 11]. This trimodal behavior cannot be captured by the β density which is at best suitable for producing bimodal distributions.

4 Appendix II

This appendix has been provided by Mr. Craig Steinberger and Mr. Thomas Vidoni. Mr. Steinberger is currently being partially supported under this grant.

Problem Description

The flow under investigation consists of a spatially developing, two-dimensional, planar jet flame. The fuel, F, discharges from the inner higher speed jet to a co-flowing lower velocity oxidizer, O, stream. The flow evolves spatially in the streamwise direction (x), and impermeable boundary conditions are imposed in the cross-stream direction (y). The computational procedure involved in DNS is the same as that employed in [12]. This involves the discretization of the complete Navier-Stokes equations as well as the applicable Fickian chemical species conservation equations. This discretization is based on a *two-four* (second order accurate in time, and fourth-order truncation in space) compact parameter finite difference scheme. This scheme has been developed and made fully operational in [13] and is utilized in the context of the *SPARK* computer code developed in [14]. A generalized single step Arrhenius exothermic chemistry model of the form $F + O \rightarrow$ Products + Heat is assumed. This kinetic mechanism is simple enough to allow an efficient treatment via DNS, and yet it is capable of capturing some of the important non-equilibrium effects associated with combustion. All the species involved in this reaction are assumed to be thermodynamically identical, and the values of the physical transport parameters are assumed to be invariant with temperature. The flow field is initialized with a top hat streamwise velocity profile with a low amplitude random forcing at the jet entrance. The magnitudes of the forcing frequency and the phase shifts between the different components of the forcing eigenfunctions are selected randomly from a seed with a top hat probability frequency and with specified values of the mean and the rms. This random specification of the frequency and the phase shift is intended to mimic the influence of turbulence in an otherwise deterministic simulation. The amplitudes of the perturbation are chosen so that the maximum value of the turbulent intensity at the inflow is no more than 5%.

The parameters influencing the rate of reactant conversion in this setting are the Damköhler number, the Zeldovich number, the Reynolds number, the heat release parameter, the convective Mach number and the Prandtl/Schmidt numbers. Based on our earlier findings [15, 12], in the range of parameters considered the Reynolds number does not have a significant effect. Therefore, the influences of this parameter and those of the Peclet and the Schmidt numbers are not investigated. The magnitudes of the Zeldovich number and the heat release parameter are held constant in all the simulations. In the computational formulation, the full compressible form of the transport equations are considered. However, the range of the convective Mach numbers considered is not very large; therefore, many of the physical issues associated with high speed combustion [14, 16, 12] are not addressed.

With available computational resources, numerical experiments with a resolution of 245 (in x) $\times$165 (in y) mesh are possible. This resolution is sufficient provided that an appropriate grid generation procedure with a non-uniform mesh and with a heavy concentration of grid points near the regions of maximum instantaneous shear is utilized [14, 15, 12]. With this configuration, it is possible to perform simulations with moderate values of the Reynolds, Peclet, Damköhler and Zeldovich numbers within a domain $13\frac{1}{3}D > x > 0$, $3\frac{1}{3}D > y > -3\frac{1}{3}D$, where D denotes the width of the jet at the inflow. With the numerical resolution attained, it was possible to perform simulations with a Reynolds number of 3×10^4 based on the velocity difference between the two jet streams at the inflow $(U_F - U_O)$, the jet width (D), and the density at the inlet. The magnitudes of the Prandtl and the Schmidt numbers were assumed to be equal to unity, resulting in an identical value for the Reynolds and the Peclet numbers. The velocity ratio between the two streams is $\frac{U_F}{U_O} = \frac{1}{2}$. A complete typical simulation requires about 6 hours of CPU time on a CRAY-2 supercomputer.

In order to show the effects of exothermicity, simulations are performed of both a heat releasing (flame D) and a non-heat releasing flame (Flame A). A comparison between the product thickness of this two flames is made in Fig. 6. This figure indicates a higher rate of product formation for the case of exothermic reaction. This observation is not consistent with any of the previous DNS [17, 12] or experimental [18, 19] results. Based on our observation, we recommend that the effects of exothermicity be assessed

by means of laboratory measurements. These measurements must involve a reacting system whereby the rate of reaction conversion is temperature dependent and in which the large scale mixing intensity is not significantly affected by the heat release. It is important to note that the issue would not be resolved by a mere comparison of the mixing characteristics between a reacting and a non-reacting layer. An appropriate analysis requires the consideration of two reacting systems with the same hydrodynamic characteristics but with different magnitudes of the enthalpy of combustion. The extent of validity of our conclusion under more complex chemistry models can be determined by these experiments.

Figure Captions

Figure 1. Time sequence of contour plots of instantaneous product concentration.

Figure 2. Cross stream variation of mean product concentration ($< C_p >$) from the DNS and the model; (a) $x/\delta = 11$, (b) $x/\delta = 22$.

Figure 3. Cross stream variation of the negative of the unmixedness from the DNS and the model; (a) $x/\delta = 11$, (b) $x/\delta = 22$.

Figure 4. Streamwise variation of total product (T_p) from the DNS and the model.

Figure 5. Cross stream variations of the third moment (μ_3) of the Shvab-Zeldovich variable from the DNS and the model; (a) $x/\delta = 11$, (b) $x/\delta = 22$.

Figure 6. Cross stream variations of fourth moment (μ_4) of the Shvab-Zeldovich variable from the DNS and the model; (a) $x/\delta = 11$, (b) $x/\delta = 22$.

Figure 7. The streamwise variation of the product thickness under both non-heat releasing (Flame A) and heat releasing (Flame D) conditions.

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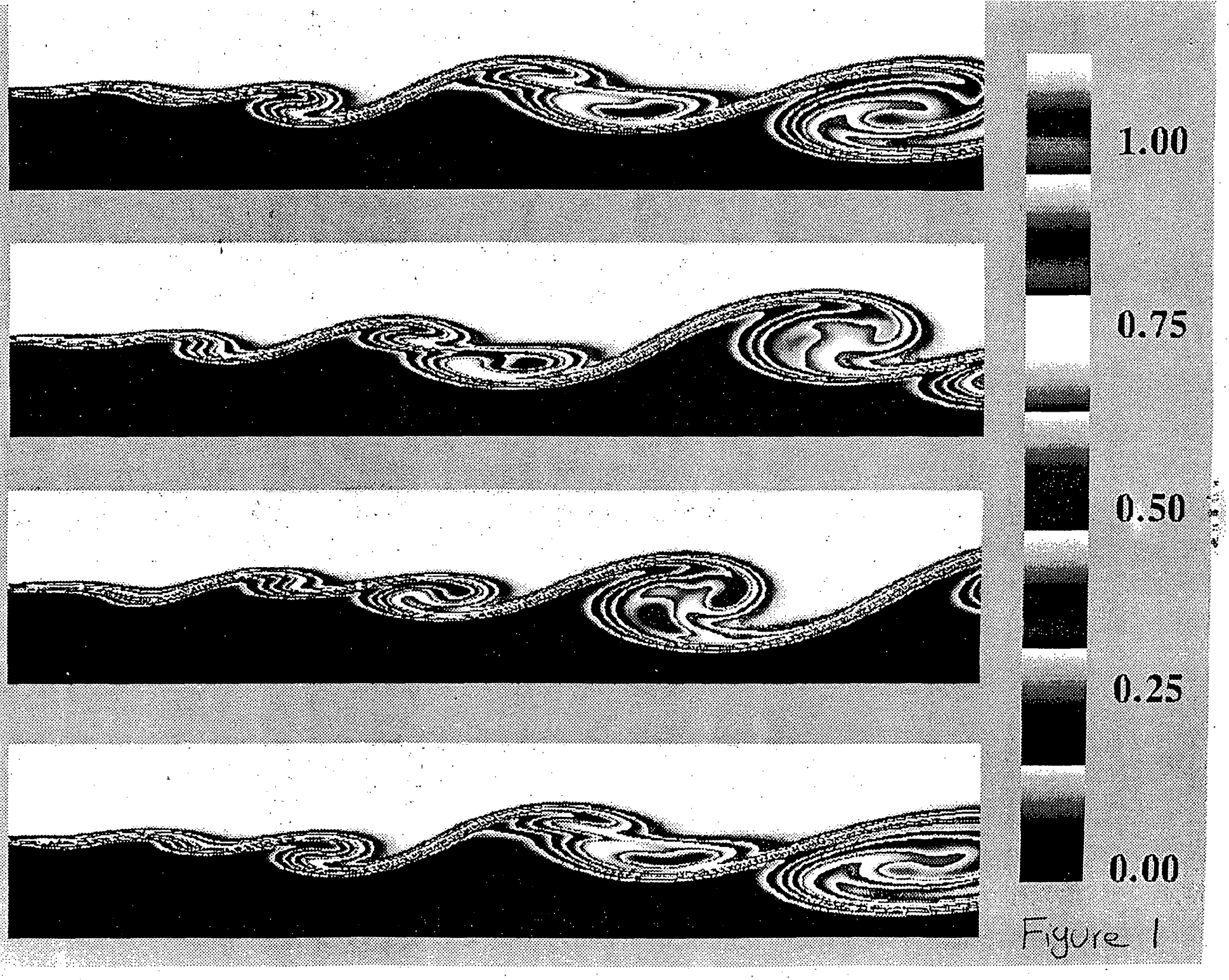

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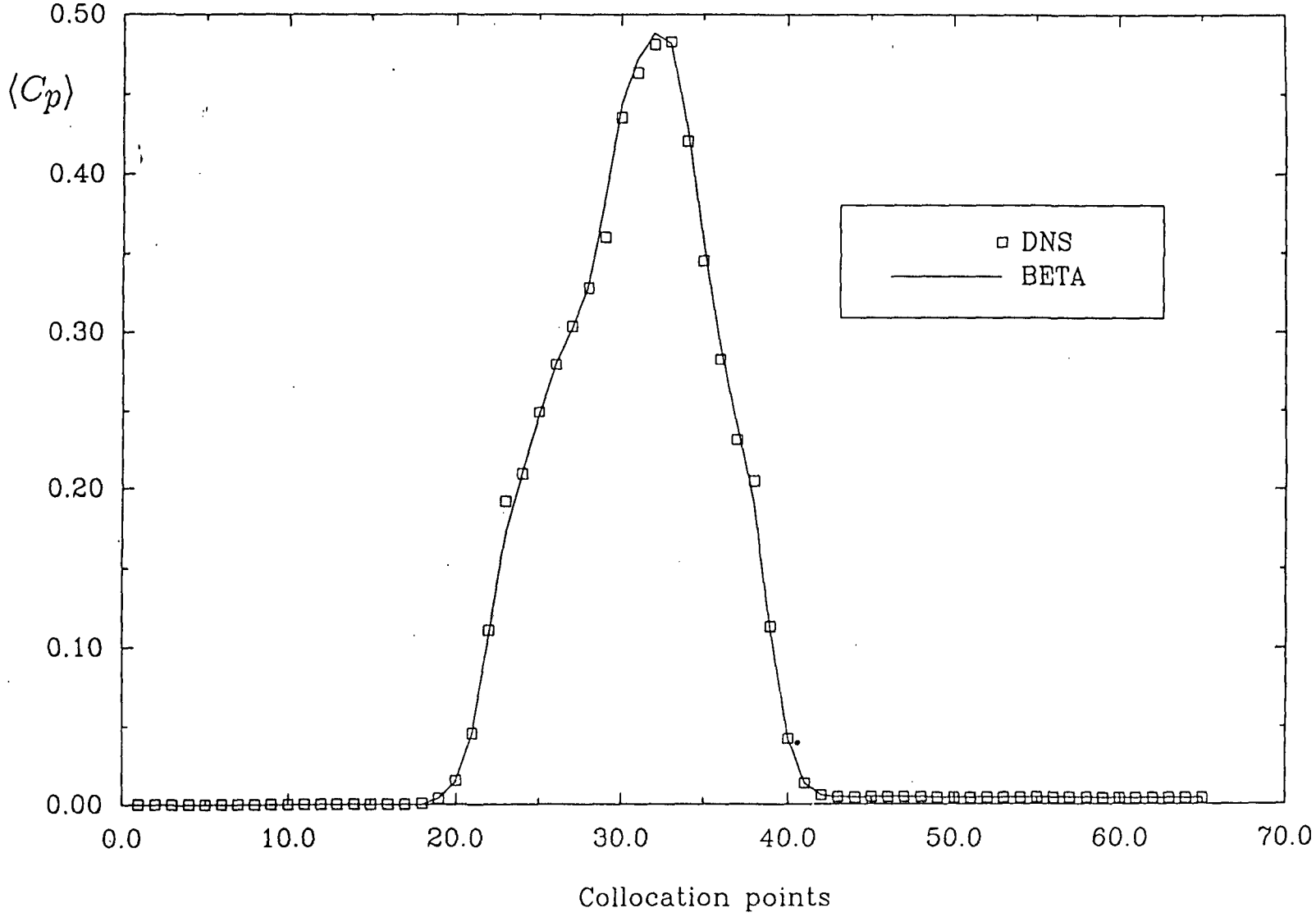
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DNS
BETA

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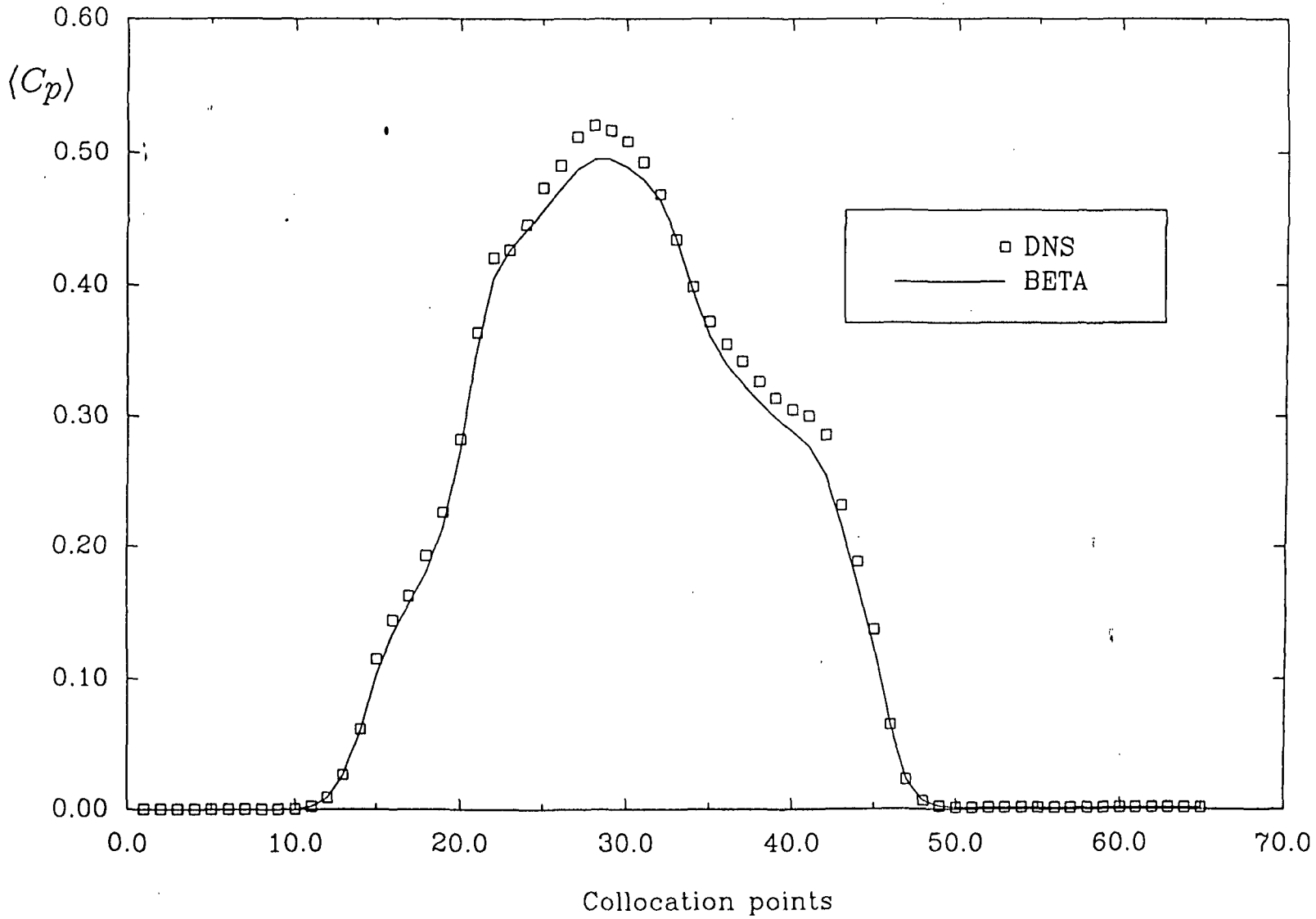
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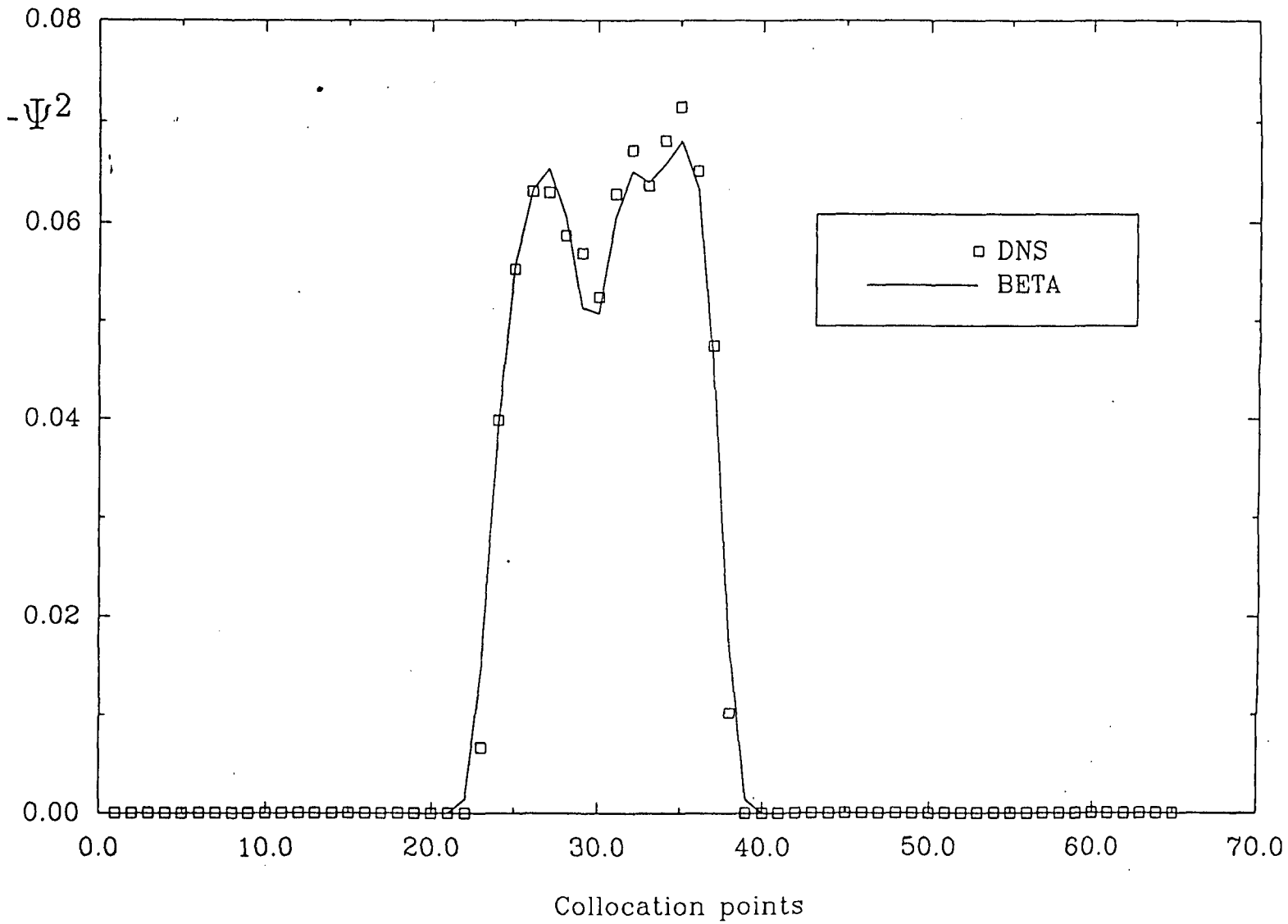
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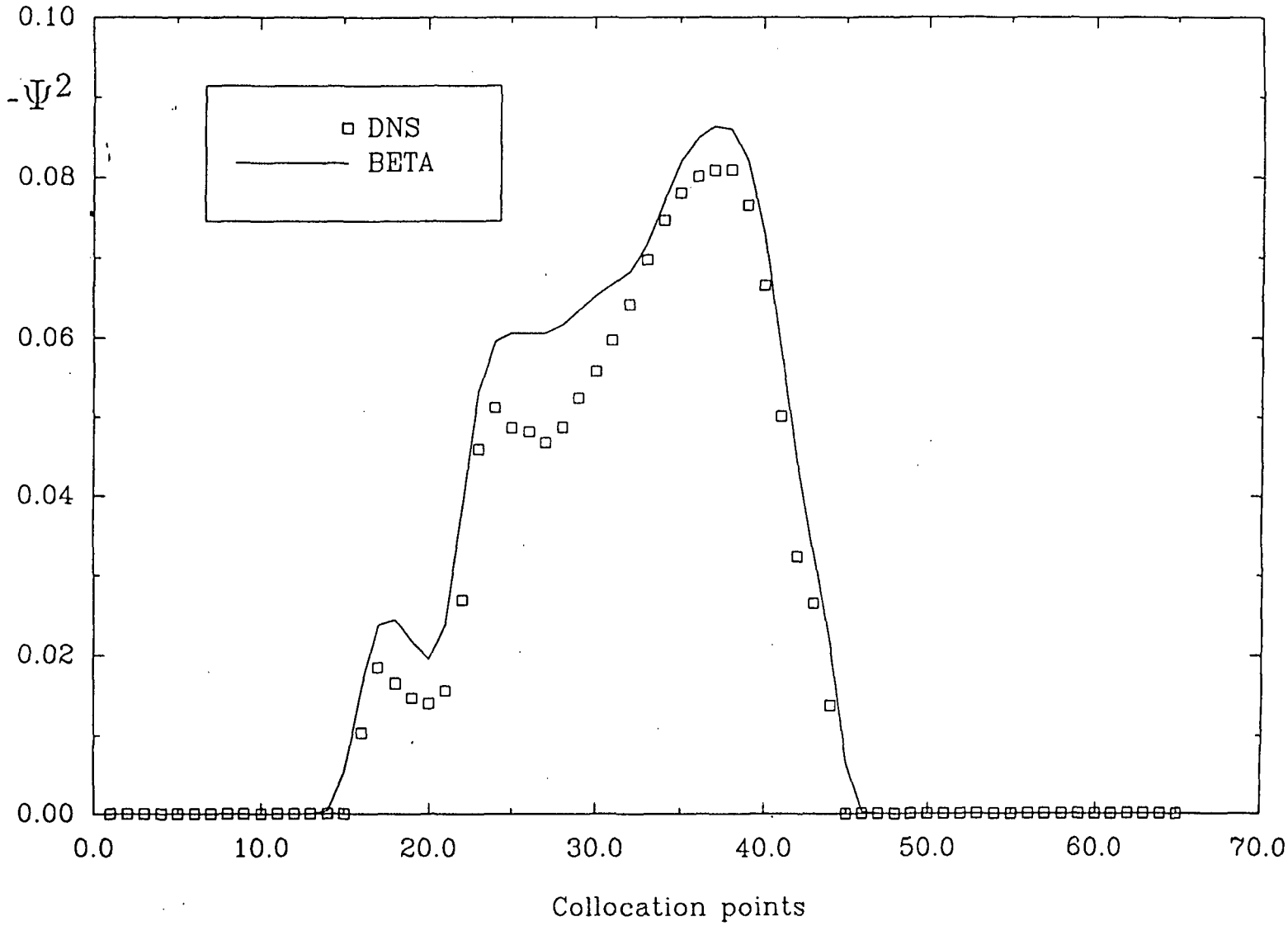
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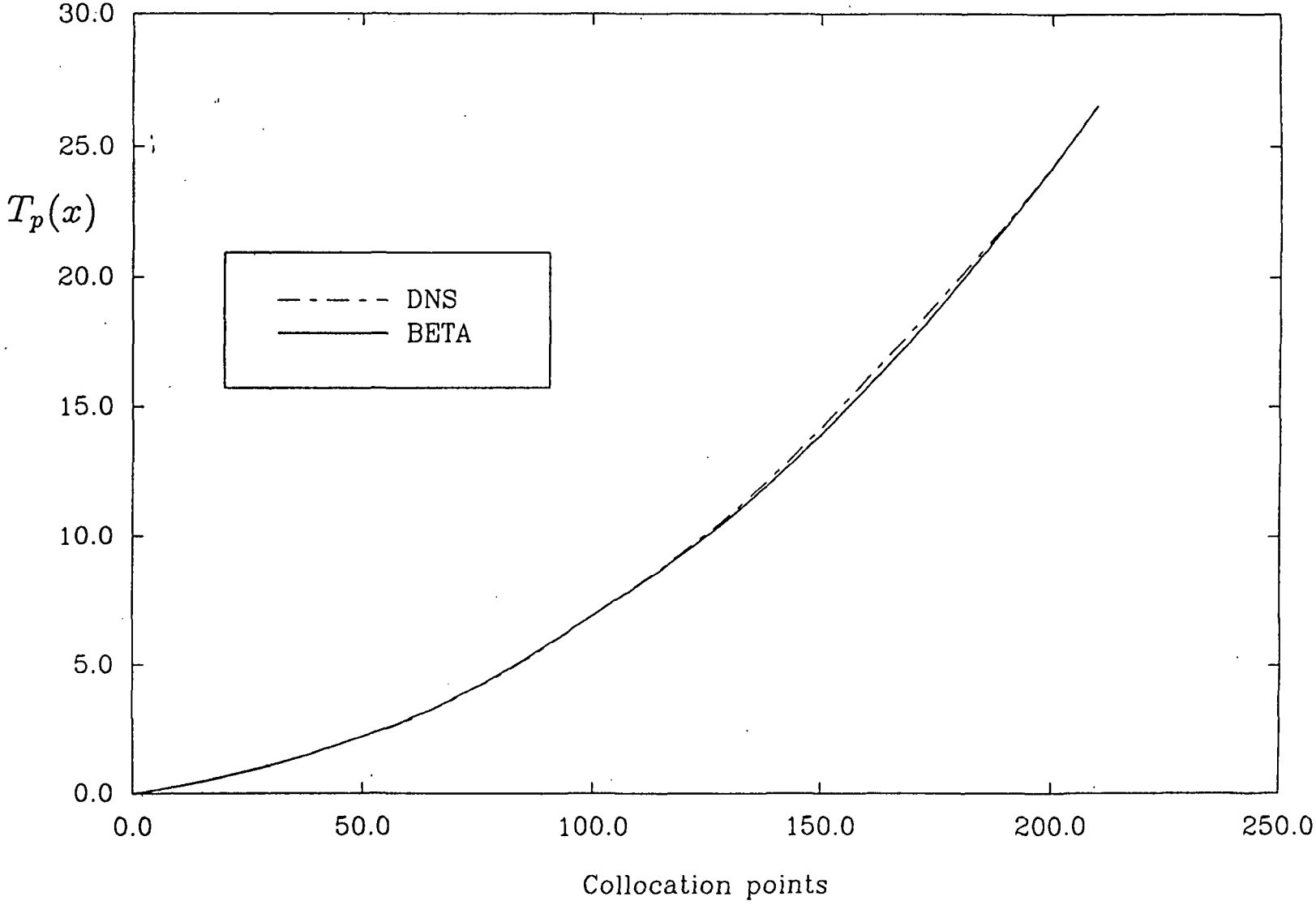
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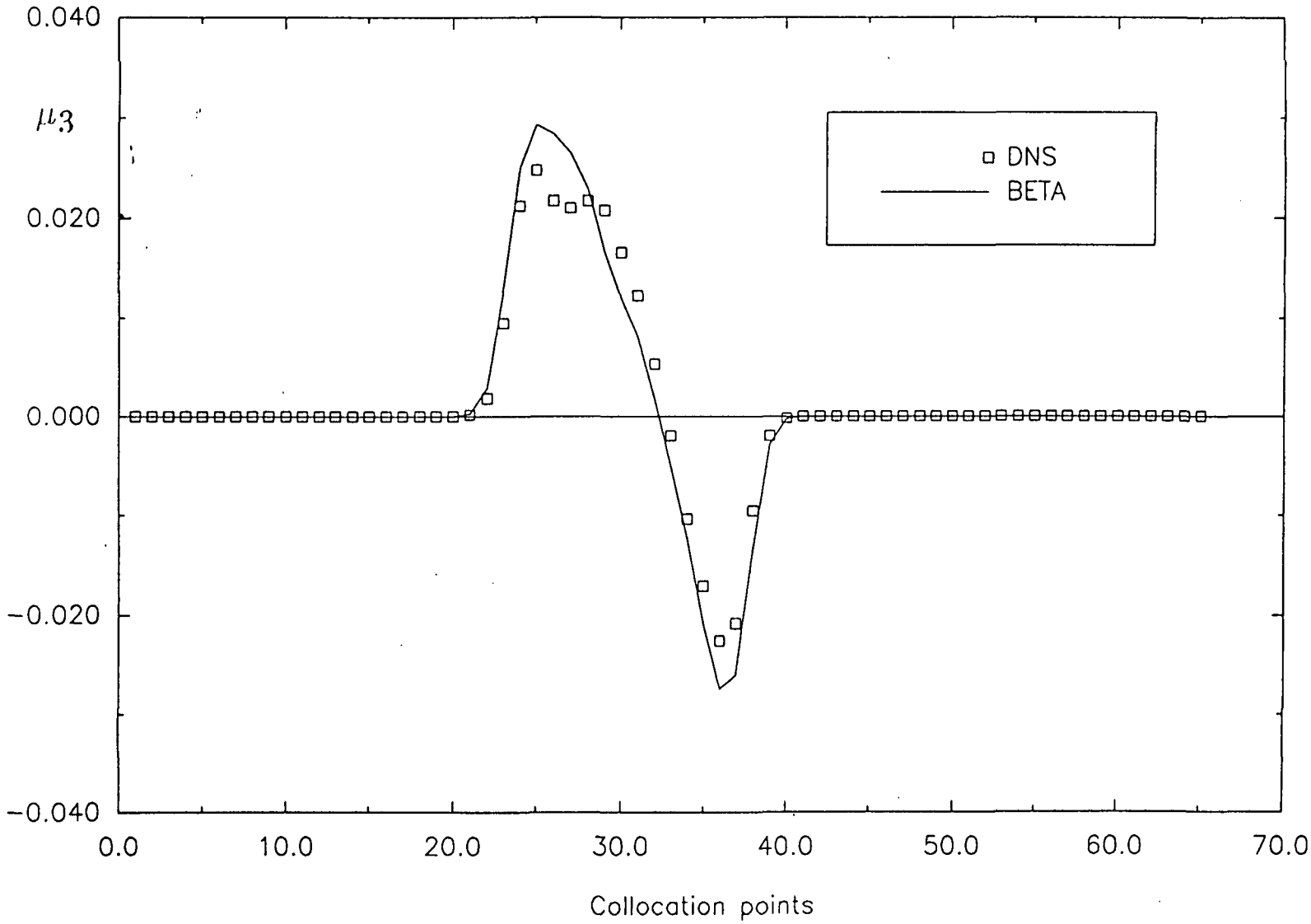
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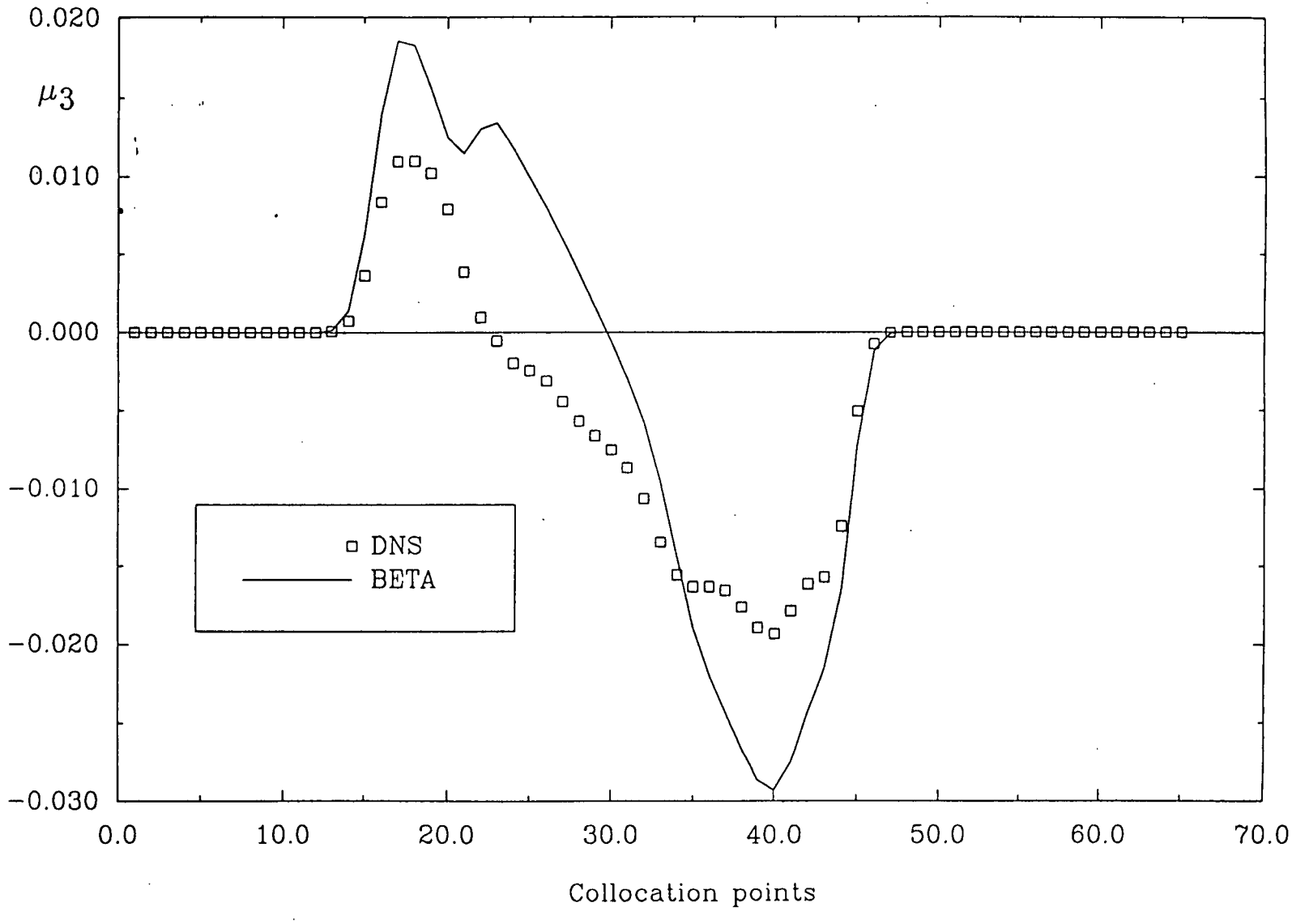
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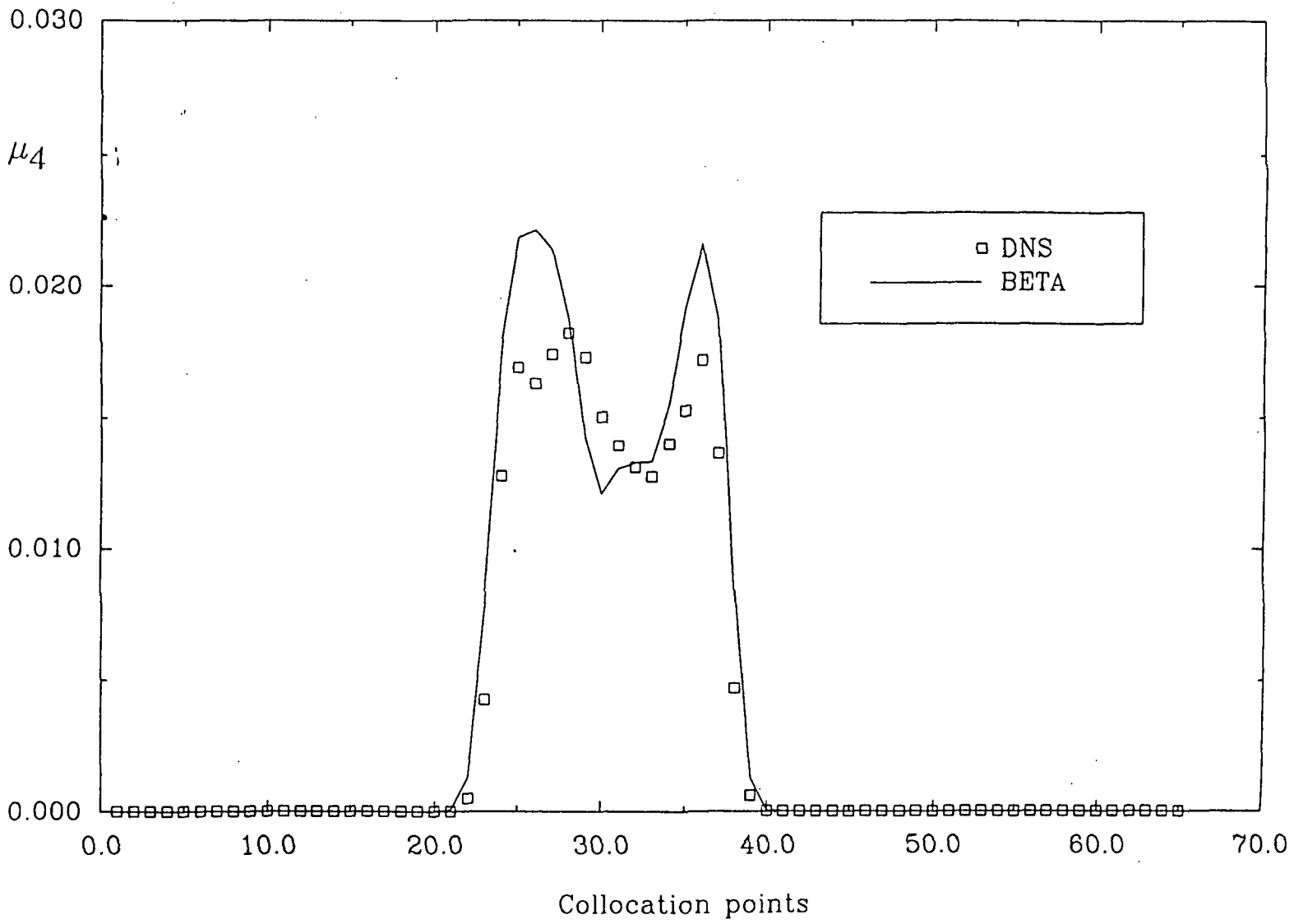
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BETA

Figure 6(a)

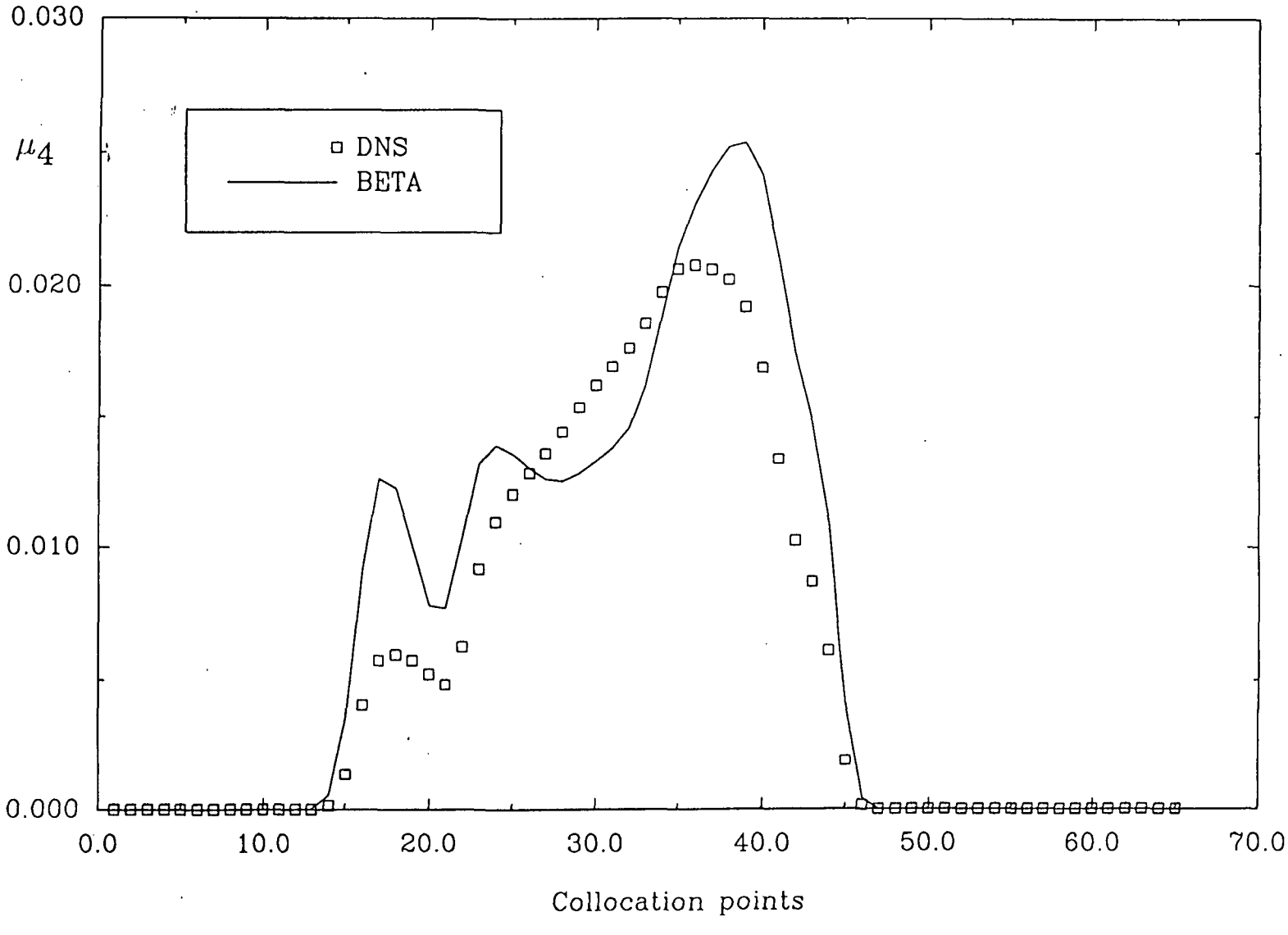
0.030
μ_4
0.020
0.010
0.000
DNS
BETA
0.0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
Collocation points

Figure 6(b)

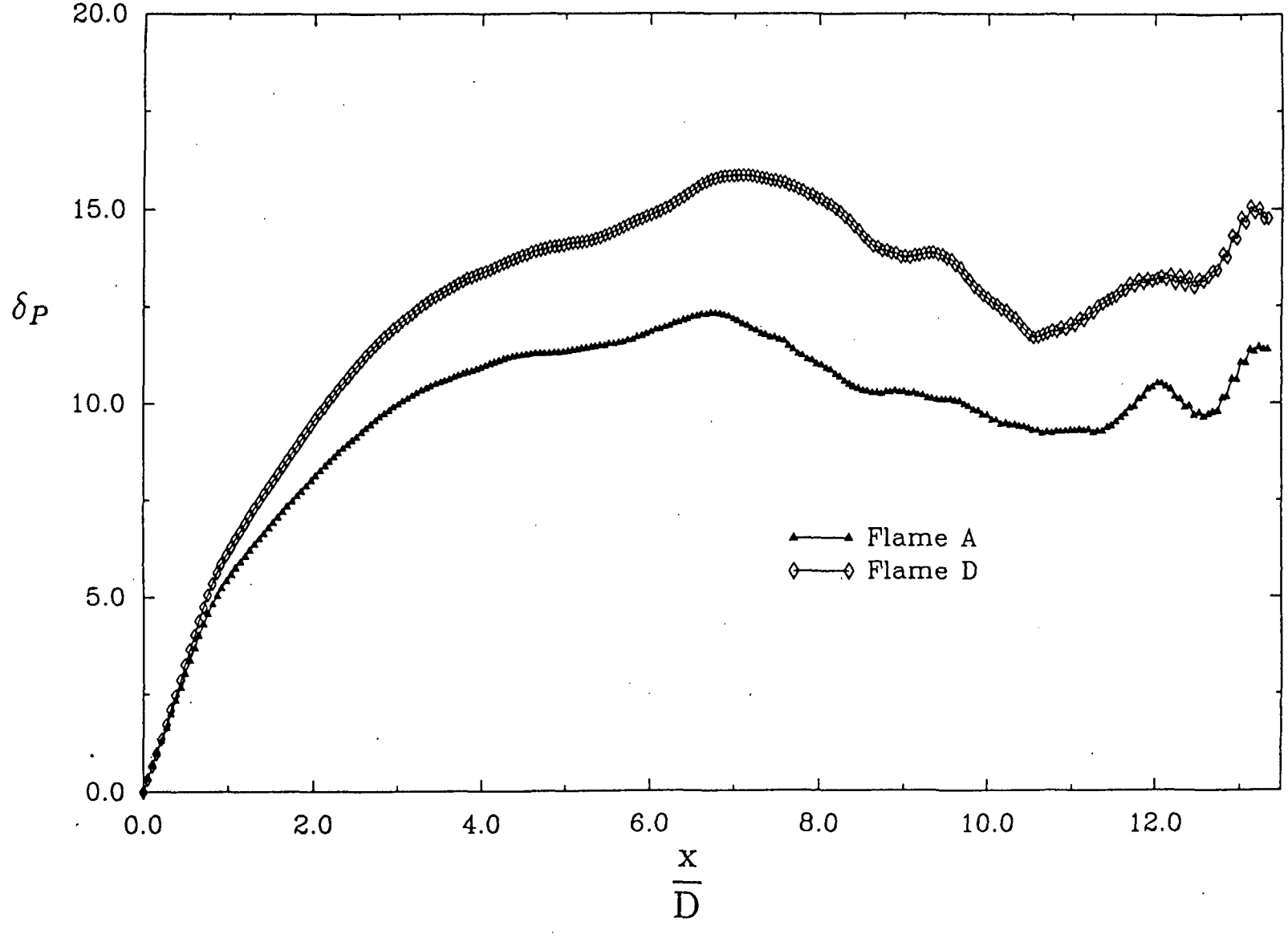

Figure 7