Application of finite element method to General Dynamic Equation of Aerosols – comparison with classical numerical approximations

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INTRODUCTION

Aerosols play a major role in many atmospheric processes. Currently the global climate models use only crude approximations of the aerosol dynamics; this is mainly because of the high computational demand of aerosol models when combined with global models.

Behavior of aerosol number distributions can be described with the General Dynamic Equation of aerosols, GDE, which is integro-partial differential equation:

$$\frac{\partial n(v_\mathrm{p},t)}{\partial t} = -\frac{\partial}{\partial v_\mathrm{p}}[I_0(v_\mathrm{p})n(v_\mathrm{p},t)] + \frac{1}{2}\int_0^{v_\mathrm{p}} \beta(v_\mathrm{p}-w_\mathrm{p},w_\mathrm{p})n(v_\mathrm{p}-w_\mathrm{p},t)n(w_\mathrm{p},t)\mathrm{d}w_\mathrm{p} - n(v_\mathrm{p},t)\int_0^{\infty}\beta(v_\mathrm{p},w_\mathrm{p})n(w_\mathrm{p},t)\mathrm{d}w_\mathrm{p} + S(v_\mathrm{p},t) - R(v_\mathrm{p},t)n(v_\mathrm{p},t),$$

where t is time, v_p is the particle volume, $n(v_\mathrm{p},t)$ is the aerosol number distribution, $I_0(v_\mathrm{p})$ is the growth/evaporation rate and $\beta(v_\mathrm{p},w_\mathrm{p})$ is the coagulation kernel function. In this formulation, nucleation and possible emissions are included in the source term $S(v_\mathrm{p},t)$, while dry and wet deposition can be included in the removal rate $R(v_\mathrm{p},t)$ [1]. The finite element method is tested in aerosol dynamic modeling and compared to the commonly used sectional method.

FINITE ELEMENT METHOD FOR THE GENERAL DYNAMIC EQUATION OF AEROSOLS

In order to apply the FEM, the GDE is written in variational form for the finite interval, where $v_{\min}$ and $v_{\max}$ are the minimum and maximum particle sizes respectively. In addition, following initial and boundary condition are introduced

$$n(v_{\min},t) = n_{\min}(t),$$
$$n(v_\mathrm{p},0) = n_0(v_\mathrm{p}).$$

Furthermore, piecewice linear basis and test functions are used. With these conditions and functions, the following finite element matrix form is obtained [2]

$$A\bar{n}'(t) = G\bar{n}(t) + \begin{bmatrix} \bar{n}^{\mathrm{T}}(t)(B^0-C^0)\bar{n}(t) \\ \bar{n}^{\mathrm{T}}(t)(B^1-C^1)\bar{n}(t) \\ \vdots \\ \bar{n}^{\mathrm{T}}(t)(B^{N+1}-C^{N+1})\bar{n}(t) \end{bmatrix} + AS(t) - AR(t)\bar{n}(t),$$

where

$$A(i,j) = \int_{v_{\min}}^{v_{\max}} \phi_i(v_\mathrm{p})\xi_j(v_\mathrm{p})\mathrm{d}v_\mathrm{p}$$
$$B^j(i,k) = \frac{1}{2}\int_{v_{\min}}^{v_{\max}}\left[\int_{v_{\min}}^{v_\mathrm{p}-v_{\min}} \beta(v_\mathrm{p}-w_\mathrm{p},w_\mathrm{p})\phi_i(v_\mathrm{p}-w_\mathrm{p})\phi_k(w_\mathrm{p})dw_\mathrm{p}\right]\xi_j(v_\mathrm{p})\mathrm{d}v_\mathrm{p},$$
$$C^j(i,k) = \int_{v_{\min}}^{v_{\max}}\left[\int_{v_{\min}}^{v_{\max}} \beta(v_\mathrm{p},w_\mathrm{p})\phi_k(w_\mathrm{p})\mathrm{d}w_\mathrm{p}\right]\phi_i(v_\mathrm{p})\xi_j(v_\mathrm{p})\mathrm{d}v_\mathrm{p},$$
$$G(i,j) = \int_{v_{\min}}^{v_{\max}} I_0(v_\mathrm{p})\phi_i(v_\mathrm{p})\frac{\partial \xi_j(v_\mathrm{p})}{\partial v_\mathrm{p}}\mathrm{d}v_\mathrm{p},$$
$$R(t) = \mathrm{diag}[R_0(t), R_1(t), \cdots, R_N(t), R_{N+1}(t)],$$
$$S(t) = [S_0(t), S_1(t), \cdots, S_N(t), S_{N+1}(t)]^{\mathrm{T}}.$$

PETROV-GALERKIN FINITE ELEMENT METHOD

If only condensation is affecting the aerosol number distribution, the GDE becomes a hyperbolic partial differential equation which are notoriously unstable. Therefore, an stabilizing unwinding scheme, Petrov-Galerking finite element method (PGFEM), is applied. In the PGFEM, the test function is

$$\xi_j(v) = \phi_j(v) + \frac{3}{2}\epsilon(\sigma_j(v) - \sigma_{j+1}(v)),$$

where $\epsilon \in [0,1]$ is the so-called upwinding factor and $\sigma_j(v)$ is a quadratic polynomial of the form

$$\sigma_j(v) = \begin{cases} \frac{4}{h_j^2}(v-v_{j-1})(v_j - v), & \text{when } v \in [v_{j-1}, v_j] \\ 0, & \text{otherwise,} \end{cases}$$

where $h_j = v_j - v_{j-1}$.

CONCLUSIONS AND FUTURE WORK

The results show that in the case of the condensation equation, the FEM and PGFEM are more accurate than the sectional method. The PGFEM reduced numerical oscillation that appeared in the numerical approximation when the number of elements was low. In the cases where the evolution of the aerosol number distribution driven by both condensation and coagulation processes, the FE based approximation methods were more accurate than the sectional method. FEM and PGFEM are viable methods for estimating the temporal evolution of the aerosol number distribution. In the future, it might be possible to implement the FE based approximation methods into the climate models to improve accuracy and certainty of modeling, especially, in the condensation dominated scenarios.

RESULTS

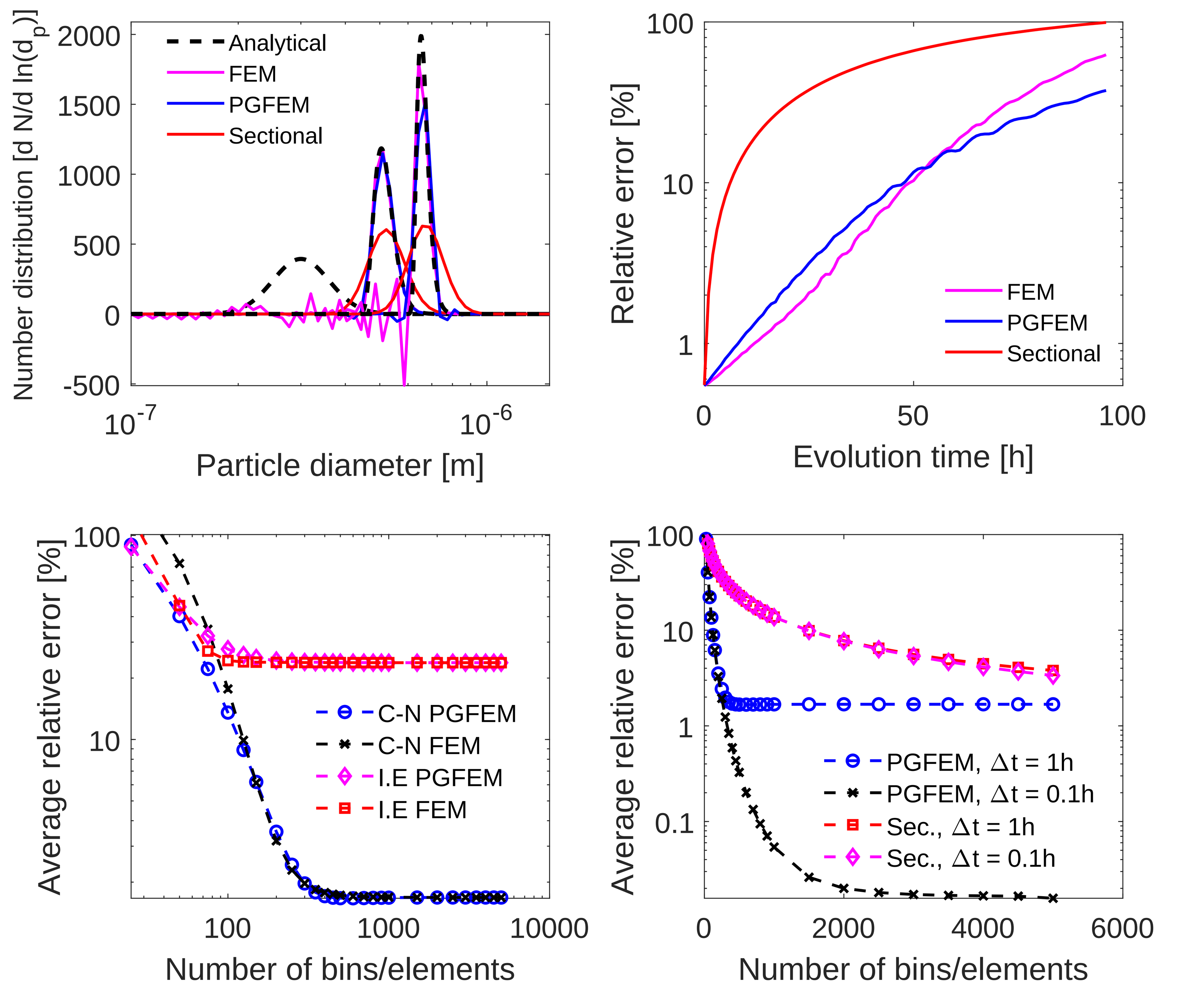

FIGURE 1: CONDENSATION TEST CASE. FEM, PGFEM, AND SECTIONAL METHOD ARE COMPARED (TOP LEFT AND TOP RIGHT). TEMPORAL DISCRETIZATION SCHEMES FOR FEM AND PGFEM ARE COMPARED (BOTTOM LEFT). ACCURACY OF ESTIMATION METHODS COMPARED WITH VARIOUS DISCRETIZATIONS (BOTTOM RIGHT).

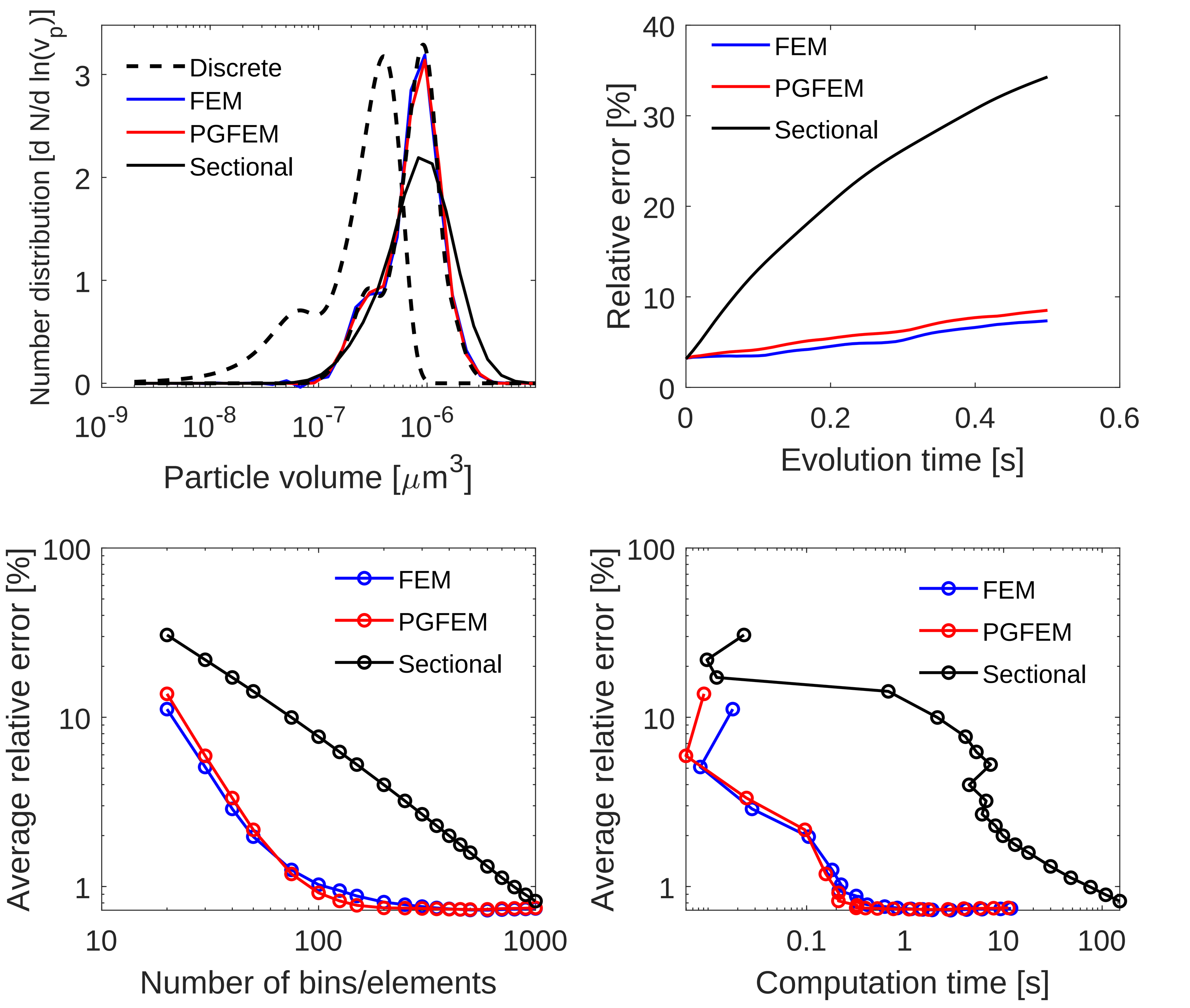

FIGURE 2: GDE WITH SIZE DEPENDENT COAGULATION KERNEL. FEM, PGFEM AND SECTIONAL METHOD ARE COMPARED (TOP LEFT AND TOP RIGHT). ACCURACY OF APPROXIMATION WITH VARIOUS DISCRETIZATIONS ARE COMPARED (BOTTOM LEFT). THE AVERAGE RELATIVE ERROR PLOTTED AS A FUNCTION OF CORRESPONDING COMPUTATION TIME (BOTTOM RIGHT).

REFERENCES AND ACKNOWLEDGMENTS

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