Defect corrected averaging for parabolic PDEs

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We consider parabolic partial differential equations with highly oscillatory source terms. The timescale of the problem is assumed to be much larger than the timescale of the oscillation. Resolution of the smallest timescale constitutes a strong restriction on the stepsize of time integration method. Averaging techniques like stroboscopic averaging have been developed to overcome this restriction. In case of parabolic equations these techniques are of limited advantage. We have developed defect corrected averaging techniques that allow timesteps taylored to the timescale of diffusion. They are based on Krylov subspace iterations for the abstract solution operator of the system.

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1 Introduction

Differential equations with a highly oscillatory forcing term constitute a challenging problem for numerical time integrators. A variety of methods has been developed to treat these problems without resolving the microscale oscillations, among them the heterogeneous multiscale framework [1] as well as averaging concepts like stroboscopic averaging [2], etc. In the concept of stroboscopic averaging the oscillatory solution is approximated at stroboscopic points by the solution of an averaged system. The righthand side of the averaged system is approximated by finite difference formulas. In contrast to that we use averaged source terms in combination with a defect correction to derive an averaged system that approximates the exact solution in the stroboscopic points $t = N\varepsilon$.

2 Averaging of oscillatory sources

We consider here parabolic initial-boundary value problems with oscillatory sources. These source terms are periodic with period length ε . Discretization in space using finite elements or finite differences leads to a system of ordinary differential equations for $y(t) \in W_h$, W_h being the discretized function space.

$$y'(t) = Ly(t) + f(t).$$
 (1)

The sources are assumed to be periodic with period length ε , i.e. $f(t + \varepsilon) = f(t)$. Note, a finite element discretization would result in My' = Ly + f, but multiplying by M^{-1} restores again the assumed form which simplifies the analysis below.

We are interested in the solution on a timescale $t_e \gg \varepsilon$ ranging over many periods without resolving the micro scale in every interval of length ε . A first step is to average the sources over an interval of length ε . We define $\hat{f} = \frac{1}{\varepsilon} \int_0^{\varepsilon} f(t) dt$ and approximate the problem by $y'(t) = Ly(t) + \hat{f}$.

3 Defect corrected averaging

Instead of simple averaging a more accurate approximation at stroboscopic points $t = N\varepsilon$, $N \in \mathbb{N}$ is available where the defect of the averaging procedure is approximated and used as a correction term.

Let $S(t_0, t_1, y_0, f)$ denote the solution operator of the differential equation (1), i.e. for y'(t) = Ly(t) + f(t), $y(t_0) = y_0$, we have $y(t_1) = S(t_0, t_1, y_0, f)$.

Whenever $f(t) = f_c$ is constant in time, the solution operator $S_c(0, t, y_0, f_c)$ is explicitly given by

$$S_c(0,t,y_0,f_c) = \exp(tL)y_0 + t\phi_1(tL)f_c,$$
(2)

where the matrix function ϕ_1 is defined by $\phi_1(z) = (\exp(z) - 1)/z$. In the general case the solution operator of (1) is given by the integral expression

$$S(0, t, y_0, f) = \exp(tL)y_0 + \exp(tL) \int_0^t \exp(-\tau L)f(\tau)d\tau.$$
(3)

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The solution of (1) at the stroboscopic points $t = N\varepsilon$ is given by

$$y(t) = \exp(tL)y_0 + \exp(tL)\sum_{k=0}^{N-1} \exp(-k\varepsilon L) \int_0^\varepsilon \exp(-\tau L)f(\tau)d\tau$$
(4)

$$=\exp(tL)y_0 + t\phi_1(tL)\left(\varepsilon\phi_1(\varepsilon L)\right)^{-1}\int_0^\varepsilon\exp(-\tau L)f(\tau)d\tau.$$
(5)

Thus $S(0, t, y_0, f) = S(0, t, y_0, \cdot) \circ S_c(0, \varepsilon, 0, \cdot)^{-1} \circ S(0, \varepsilon, 0, f)$ for $t = N\varepsilon$. This suggests the following procedure: given a periodic source f(t), we find the constant source $f_c(t) = f_c = S_c(0, \varepsilon, 0, \cdot)^{-1} \circ S(0, \varepsilon, 0, f)$. f_c is defined by the property

$$S(0,\varepsilon,0,f_c) = S(0,\varepsilon,0,f),$$
(6)

i.e., the constant source f_c generates the same flow as the varying source f(t) in $[0, \varepsilon]$. This constant source is used to compute the solution at selected stroboscopic points $N_i \varepsilon$. In the problem with source f_c the small time scale is eliminated, we can use macro time steps $H \ll \varepsilon$ tailored to the global time scale and accuracy requirements of the averaged problem.

We point out, that for large scale problems the computation of exp, ϕ_1 is costly and only possible by approximations. For the matrix exponential we refer to the classic paper of Moler and van Loan, [3]. For functions like ϕ_1 or ϕ_1^{-1} it is even more complicated. Our procedure works without utilizing these matrix function – we use only an approximate solution operator available by suitable numerical integration procedures.

We have to determine a constant source f_c with $S(0, \varepsilon, 0, f_c) = S(0, \varepsilon, 0, f)$. This constitutes a linear equation Ax = bin the vector space W_h , where $x = f_c$ is the unknown, $b = S(0, \varepsilon, 0, f)$ is the righthand side, and the linear operator A is the solution operator of (1). The righthand side b is evaluated by a suitable time integrator. The matrix A is not explicitly available, but we can compute Ax by a time integrator applied to y' = Ly + x, y(0) = 0 in the interval $[0, \varepsilon]$. This is the standard situation to apply a Krylov solver to the linear equation. Here, we apply the GMRES method [4]. The convergence of the iterative solver is greatly improved, if the approach is combined with simple averaging, i.e. f_c with $S(0, \varepsilon, 0, f_c) = S(0, \varepsilon, 0, f - \hat{f})$ is approximated. Note, that each Krylov iteration requires the solution of the problem on the micro scale of length ε . Nevertheless, these have to be executed only once as a preprocessing step. Afterwards, the problem can be solved using the constant source f_c (resp. $f_c + \hat{f}$) with a few iteration steps on $[0, t_e]$.

4 Numerical results

We tested the defect correction scheme depicted above using an equidistant finite difference discretization of an 1:4 rectangle. The periodic source results from a moving contact of length 1 at the lower boundary. The contact moves along the lower side with a sinoidal movement. We apply zero flux boundary conditions outside the contact, and a constant flux inside the contact. After 100 periods, the temperature increased by 12 Kelvin and the sinoidal profile remains clearly visible, see left of Figure 1. In the right we show the errors in the point (3.2, 0) for simple averaging as well as for defect corrected averaging. The rows correspond to different macro step sizes H where a second order Rosenbrock method is used as macro time integrator. Simple averaging gives only a rough approximation to the solution, whereas the defect corrected version is up to two orders of magnitude more accurate. The procedure takes 6 Krylov iterations as a preprocessor.



Fig. 1: Left: Solution at $t_e = 100\varepsilon$. Right: errors in simply averaged and defect corrected solution.

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