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EXPONENTIAL INTEGRATORS FOR QUANTUM-CLASSICAL MOLECULAR DYNAMICS

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Abstract.

We study time integration methods for equations of mixed quantum-classical molecular dynamics in which Newtonian equations of motion and Schrödinger equations are nonlinearly coupled. Such systems exhibit different time scales in the classical and quantum evolution, and the solutions are typically highly oscillatory. The numerical methods use the exponential of the quantum Hamiltonian whose product with a state vector is approximated using Lanczos' method. This allows time steps that are much larger than the inverse of the highest frequencies.

We describe various integration schemes and analyze their error behaviour, without assuming smoothness of the solution. As preparation and as a problem of independent interest, we study also integration methods for Schrödinger equations with time-dependent Hamiltonian.

AMS subject classification: 65L05, 65L70, 65M12, 65M20.

Key words: Numerical integrator, oscillatory solutions, Schrödinger equation, quantum-classical coupling, error bounds, stability.

1. Introduction.

The inclusion of quantum behaviour in molecular dynamics simulations is a topic of considerable current interest; see the contributions in the recent volume [4]. Since a full quantum simulation of molecules is out of question, mixed quantum-classical models offer feasible alternatives. A widely used model couples Newtonian equations of motion and Schrödinger equations in the following way:

Mψ'' = -∇_y^2(ψ^* H(y) ψ), iψ' = H(y)ψ.

Here, y denotes the positions of the classical particles and ψ represents the wave functions. M is the mass matrix and H(y) is the Hamilton operator—or as will be assumed here—its spatial discretization. The typical situation is that H(y) is a sum of a (discretized) negative Laplacian and a position-dependent

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Summary. We study time integration methods for equations of mixed quantum-classical molecular dynamics in which Newtonian equations of motion and Schrödinger equations are nonlinearly coupled. Such systems exhibit different time scales in the classical and quantum evolution, and the solutions are typically highly oscillatory. The numerical methods use the exponential of the quantum Hamiltonian whose product with a state vector is approximated using Lanczos' method. This allows time steps that are much larger than the inverse of the highest frequencies. We describe various integration schemes and analyze their error behaviour, without assuming smoothness of the solution. As preparation and as a problem of independent interest, we study also integration methods for Schrödinger equations with time-dependent Hamiltonian.

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1. Introduction.

Low rank approximation of time-dependent data matrices and of solutions to matrix differential equations, an incremental-based computational approach is proposed and analyzed. In this method, the derivative is projected onto the tangent space of the manifold of rank-r matrices and the error analysis compares the result with the pointerwise best approximation in the Frobenius norm. It is shown that the approach gives locally quasi-optimal low rank approximations. Numerical experiments illustrate the theoretical results.

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1. Introduction.

Since the work of Wilkinson (1960), backward error analysis has become a well-established tool in numerical linear algebra. For the numerical treatment of ordinary differential equations its use is only very recent. The papers by Eidelit and Yoshida (1993) and Fung-Kang (1991) appear to be among the first studies on this topic. The idea is to interpret the numerical solution of the exact solution of a perturbed differential equation (the numerical solution yielding new insight into a perturbed differential equation) as the numerical solution of an ordinary differential equation.

We consider the system of ordinary differential equations

Y'(t) ∈ T_{Y(t)} M_r, such that ||Y'(t) - A(t)Y(t)|| = min

This is complemented with an initial condition, ideally Y(t_0) = X(t_0). For given dependent vector spaces. Problem (1.2) yields an initial value problem of nonlinear differential equations determining the solution of (1.2) and study the approximation properties of this approach. It is clear that Y(t) cannot always be expected to remain close to X(t). This is already seen from the example of finding a rank-1 approximation to diag(e^{-t}, e^t), where starting from t < 0 yields X(t) = Y(t) = diag(e^{-t}, 0)

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FAST CONVOLUTION FOR NONREFLECTING BOUNDARY CONDITIONS*

CHRISTIAN LUBICH¹ AND ACHIM SCHÄDLÉ²

Dedicated to Gerhard Wanner on the occasion of his 60th birthday

Abstract. Nonreflecting boundary conditions for problems of wave propagation are nonlocal in space and time. While the nonlocality in space can be efficiently handled by Fourier or spherical expansions in special geometries, the arising temporal convolutions still form a computational bottleneck. In the present article, a new algorithm for the evaluation of these convolution integrals is proposed. To compute a temporal convolution over N_t successive time steps, the algorithm requires O(N_t log N_t) operations and O(log N_t) memory. In numerical examples, this algorithm is used to discretize the Neumann-to-Dirichlet operators arising from the formulation of nonreflecting boundary conditions in rectangular geometries for Schrödinger and wave equations.

Key words: transparent boundary conditions, radiation boundary conditions, fast convolution algorithm, wave equation, Schrödinger equation

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∫_0^t f(t-τ)g(τ) dτ, 0 ≤ t ≤ T.

For concreteness, consider the example of the wave equation u_{tt} = u_{xx} + u_{yy} + u_{zz} on R^3. Suppose the solution is 2π-periodic in y and z, a situation that occurs in modeling wave propagation near extended layers. Transparent boundary conditions are required at the planes y = ±a. We consider the Fourier coefficients of the solution, u_k(x, t) with k = (k_y, k_z) ∈ Z × Z. Their Laplace transforms U_k(x, s) then satisfy the linear ordinary differential equation s^2 U_k = ∂_x U_k - |k|^2 U_k with |k|^2 = k_y^2 + k_z^2 for Re(s) > 0. This equation can be solved analytically. Retaining only the solution decaying to zero as |x| → ∞ gives U_k(x, s) = exp(-√(s^2 + |k|^2) |x ± a|) U_k(±a, s). Differentiation of this equation at x = ±a yields a relation between the transforms of the

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For concreteness, consider the example of the wave equation u_{tt} = u_{xx} + u_{yy} + u_{zz} on R^3. Suppose the solution is 2π-periodic in y and z, a situation that occurs in modeling wave propagation near extended layers. Transparent boundary conditions are required at the planes y = ±a. We consider the Fourier coefficients of the solution, u_k(x, t) with k = (k_y, k_z) ∈ Z × Z. Their Laplace transforms U_k(x, s) then satisfy the linear ordinary differential equation s^2 U_k = ∂_x U_k - |k|^2 U_k with |k|^2 = k_y^2 + k_z^2 for Re(s) > 0. This equation can be solved analytically. Retaining only the solution decaying to zero as |x| → ∞ gives U_k(x, s) = exp(-√(s^2 + |k|^2) |x ± a|) U_k(±a, s). Differentiation of this equation at x = ±a yields a relation between the transforms of the

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