Effective Methods for Propagating the Schrödinger in Time

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Many current approaches to propagating the Schrödinger in time use explicit time propagators based on Krylov approximations to propagate the solution. Our group has developed an efficient technique based on the short iterative Lanczos method. Here we suggest how that can be extended and perhaps made more efficient using an exponential time differencing approach.

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I. TIME PROPAGATION

Our group has been working on the time propagation of the Schrödinger In all of our work to date, we have employed the short iterative lanczos (SIL) method to compute the wavefunction from time t to time $t+\delta t$. This approach is based on developing a Krylov space approximation to the exponential of the Hamiltonian when it is sufficient to assume the Hamiltonian is not varying rapidly over the time step. To put it simply, we use the Krylov space vectors generated by the Lanczos method to "diagonalize" the matrix and then exponentiate. However, as I demonstrate below, this is just the zeroth order approximation of a far more general approach known as exponential time differencing (ETD). Let us look at the more general problem,

$$\begin{aligned}\left(i\frac{\partial}{\partial t}-L(x,t)\right)|\Psi(x,t)\rangle &= |F(x,t)\rangle \\ \left(i\frac{\partial}{\partial t}-L^0(x)\right)|\Psi(x,t)\rangle &= |F(x,t)\rangle + L^1(x,t)|\Psi(x,t)\rangle\end{aligned} \tag{1}$$

Next, we use,

$$\begin{aligned}&i\frac{\partial}{\partial t}\exp(iL^0t)|\Psi(x,t)\rangle \\ &\qquad = \\ &\qquad \exp(iL^0t)\left(-L^0|\Psi(x,t)\rangle + i\frac{\partial}{\partial t}|\Psi(x,t)\rangle\right)\end{aligned} \tag{2}$$

to rewrite Eq. 1 as,

$$i\frac{\partial}{\partial t}\exp(iL^0t)|\Psi(x,t)\rangle = |F(x,t)\rangle + L^1(x,t)|\Psi(x,t)\rangle \tag{3}$$

Integrating Eq. 3 from t to $t+\delta t$ yields,

$$\begin{aligned}|\Psi(x,t+\delta t)\rangle &= \exp(-iL^0\delta t)|\Psi(x,t)\rangle \\ &\quad -i\int_t^{t+\delta t}dt'\exp(-iL^0(t'-t-\delta t)\left[|F(x,t')\rangle\right. \\ &\quad \left.+L^1(x,t')|\Psi(x,t')\rangle\right]\end{aligned} \tag{4}$$

There are a few points to note for the discussion. The spatial discretization of L is accomplished using a spectral element method. Therefore, L, is sparse and structured. Thus, the matrix-vector multiplies required in finding the Krylov space vectors can be structured as a set of small, dense, matrix-vector operations that are distributed to the available processors with minimal communications between processors. Also,if the time dependence of the operator L were neglected and there was no inhomogeneity, the equation would reduce to our previous SIL approach. The current generalization enables the treatment of both inhomogeneities as well as the time dependence of the operator, if we can find ways to approximate the integral on the right hand side of Eq. 4. It is probably also worthwhile noting that if one make a Krylov approximation to the exponential for the first term, it can also be used under the integral sign to evaluate the additional terms. However, we have not gone so far as to insist that a single Krylov set of vectors would suffice to evaluate the exponential. There is still a time dependence coming from that part of operator at the beginning time of the step. One does have the option of putting *all* of the time dependent terms in L^1 but that might be extreme. The great advantage of Eq. 4 is that it might allow significantly larger timesteps than the SIL. The timestep in the SIL is controlled by the size of the eigenvalues from the Lanczos procedure and those can be large. Whether that would result in significant computational savings is clearly not easy to predict. This is a very useful generalization of the SIL which has not been well explored in the literature. The key to making ETD work is to find a useful and easily computed approximation to the integral. There have been a number of suggestions in the literature but the one that seems most accurate and easy to implement is a variant of the Runge-Kutta method. It would be interesting to hear what other think.