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On the development of a grid enabled a priori molecular simulator

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We have implemented on the production grid of EGEE GEMS.0, a demo version of our Molecular processes simulator that deals with gas phase atom diatom bimolecular
reactions. GEMS.0 takes the parameters of the potential from a data bank and carries out the dynamical calculations by running quasiclassical trajectories [1].
A generalization of GEMS.0 to include the calculation of ab initio potentials and the use of quantum dynamics is under way with the collaboration of the members of COMPCHEM [2]. In this communication we report on the implementation of quantum dynamics procedures.
Quantum approaches require the integration of the Schroedinger equation to calculate the scattering matrix SJ (E). The integration of the Schroedinger equation can be carried out using either time dependent or time independent techniques.
The structure of the computer code performing the propagation in time of the wavepacket (TIDEP)[3] for the Ncond sets of initial conditions is sketched in Fig. 1.

```
Read input data: tfin, tstep, system data ...
     Do icond = 1,Ncond
        Read initial conditions: v, j, Etr, J ...
         Perform preliminary and first step calculations
         Do t = to, tfin, tstep
             Perform the time step propagation
             Perform the asymptotic analysis to update S
             Check for convergence of the results
         EndDo t
     EndDo icond
```

Fig. 1. Pseudocode of the TIDEP wavepacket program kernel.

The TIDEP kernel shows strict similarities with that of the trajectory one (ABCtraj)
already implemented in GEMS.0. In fact, for a given set of initial conditions, the inner loop of TIDEP propagates recursively over time the wavepacket. The most noticeable difference between this and the trajectory integration is the fact that at
each time step TIDEP performs a large number of matrix operations which increase memory and computing time requests of some orders of magnitude.
The structure of the time independent suite of codes [4] is, instead, articulated in a different way. It is in fact made of a first block (ABM) [4] that generates the local
basis set and builds the coupling matrix (the integration bed) using also the basis set of the previous sector. This calculation has been decoupled by repeating for each

sector the calculation of the basis set of the previous one (see Fig. 2). This allows
to distribute the calculations on the grid. The second block is concerned with the propagation of the solution R matrix from small to large values of the hyperradius performed by the program LOGDER [4]. For this block, again, the same scheme of ABCtraj can be adopted to distribute the propagation of the R matrix at given values of E and J as shown in Fig. 3.

```
Read input data: in, fin, step, J, Emax, ...
     Perform preliminary calculations
     Do  (rho) = (rho)in + (rho)step, (rho)fin, (rho)step
         Calculate eigenvalues and surface functions for present and previous
```

(rho)
Build intersector mapping and intrasector coupling matrices

```
EndDo (rho)
```

Fig. 2. Pseudocode of the ABM program kernel.

```
Read input data: in, fin, step, ...
Transfer the coupling matrices generated by ABM from disk
Do icond = 1,Ncond
   Read input data: J, E ...
   Perform preliminary calculations
      Do (rho) = (rho)in, (rho)fin, (rho)step
          Perform the single sector propagation of the R matrix
     EndDo (rho)
EndDo icond
```

Fig. 3. Pseudocode of the LOGDER program kernel.

References

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