Example of a Potential Grid Technology application for effective kinetic equation calculations

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The Main Idea of Approach

evolution equation of the type

$$\frac{du}{dt} = Pu;$$

linear system ordinary differential equations of the type

$$\frac{dv}{dt} = Pv;$$

v - the large vector $P$ - symmetric matrix
The Equations of Nonequilibrium Kinetics

\[
Dc \left( j, t \right)/Dt = I \left( j - 1, t \right) - I \left( j, t \right)
\]

\[
I \left( j, t \right) = K \left( j, j + 1 \right)c \left( j, t \right) - K \left( j + 1, j \right)c \left( j + 1, t \right)
\]

new variables

\[
f \left( j, t \right) = c \left( j + 1, t \right)/c \left( j, t \right)a \left( j, t \right)
\]

\[a \left( j, t \right) \text{ the ratio of to rate constants } K \left( j, j + 1 \right) K \left( j + 1, j \right)\]

\[
df \left( j, t \right)/dt = \tilde{R} \left( f \left( j, t \right) \right) + H \left( j, t \right)f \left( j, t \right) + S \left( j \right)f \left( j, t \right)
\]
Some Particular Cases:
rotational nonequilibrium flows in jets and nozzles

\[
K(i, j) \rightarrow K^*(i, j) = K(i, j) + n \sum_k K(k, k + 1; i, j)c(k, t)
\]

\(n\) is the density,

\(K(k, k + 1; i, j)\) - rate constant for molecule-molecule collision

In the zero approximation we have the equation:

\[
df(j, t)/dt = -G(t)\Delta E_j f(j, t)
\]

\[
f^{(1)}(j, t) = \exp \left[ -\Delta E_j \int_0^t G(t) dt \right] \int_0^t R(f(j, t), f(j, t)_T) \exp \left[ \Delta E_j \int_0^T G(t_1) dt_1 \right] dt,
\]
Stages of the computation

- Rate constants computation,
- Rate constants parametrization,
- Approximate system evolution,
- Corrections for exact system evolution,
- Populations and averages computations
The basic principles of the Grid for kinetics calculation

- Present computer and data resources as a single virtual environment by developing a web portal on the Grid technology.
- Build an easy-to-use user web interface for providing access to these resources.
- Facilitate the sharing of results of research.
- Organize archiving of input, output, and intermediate data.
Using Grid for solution of the reactive scattering problem

• Rate constants computation,
• Rate constants parametrization,
• Determination of initial values of reduced populations,
• Determination of how far from equilibrium is the state,
• Computation of diagonal or nearequilibrium approximation,
• Computation of exact solution corrections,
• Determination of final distributions,
• Computations of averages,
• Visualization of the results.
The parallel scheme of computing process.

[Diagram with nodes and arrows illustrating the process steps:
- Rate constants calculation
- Initial distributions
- Reduced distributions
- "Diagonal" approximation evolution
- Nondiagonal corrections
- "Exact" system evolution
- Final distributions
- "Averages" computations]
Important Example

The difference between exact (solid lines) and diagonal approximation (dashed lines) populations for He-HF mixture nozzle flow.
TESTBED
Conclusions

The use of some physical considerations makes it possible:

- to derive some new algorithms for solution of the evolution equations for physical variables like distribution function
- to reduce the needed computer time orders of magnitude
- go to substantially larger number of processor
- work out approximate methods, which can be used for mass computations in technical applications.
- essentially reduce computational time in comparison with the parallel approach