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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

$$du/dt = Pu;$$

$i\, d\mathbf{v}/dt = \mathbf{P}\mathbf{v}$

linear system ordinary differential equations of the type

$$d\mathrm{v}/dt = \mathrm{Pv};$$

v - the large vector ***P*** **-** symmetric matrix

The Equations of Nonequilibrium Kinetics

$$Dc\left(\mathbf{j},t\right)/Dt = I\left(\mathbf{j}-\mathbf{1},t\right) - I\left(\mathbf{j},t\right)$$

$$I\left(\mathbf{j},t\right) = K\left(\mathbf{j},\mathbf{j}+\mathbf{1}\right)c\left(\mathbf{j},t\right) - K\left(\mathbf{j}+\mathbf{1},\mathbf{j}\right)c\left(\mathbf{j}+\mathbf{1},t\right)$$

new variables

$i\,d\mathbf{v}/dt = \mathbf{P}\mathbf{v}$

$$f\left(\mathbf{j},t\right) = c\left(\mathbf{j}+\mathbf{1},t\right)/c\left(\mathbf{j},t\right)a\left(\mathbf{j},t\right)$$

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

$$df\left(\mathbf{j},t\right)/dt = \tilde{R}\left(f\left(\mathbf{j},t\right)\right) + H\left(\mathbf{j},t\right)f\left(\mathbf{j},t\right) + S\left(\mathbf{j}\right)f\left(\mathbf{j},t\right)$$

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,

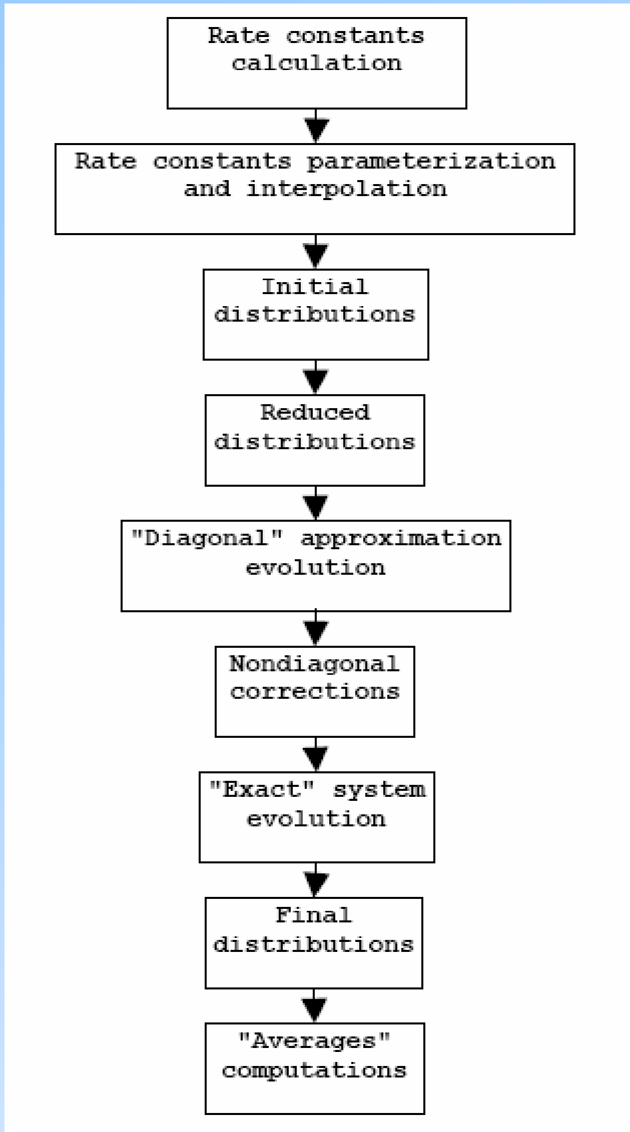
$K(k,k+1;i,j)$ - rate constant for molecule-molecule collision

In the zero approximation we have the equation:

$$df(\mathbf{j},t)/dt = -G(t)\Delta E_{\mathbf{j}} f(\mathbf{j},t)$$

$$f^{(1)}(\mathbf{j},t) = \exp\left[-\Delta E_{\mathbf{j}}\int_0^t G(t)dt\right]\int_0^t R(f(\mathbf{j},t), f(\mathbf{j},t))_T \exp\left[\Delta E_{\mathbf{j}}\int_0^T G(t_1)dt_1\right]dt,$$

Stages of the computation



- Rate constants computation,
- Rate constants parametrization,
- Approximate system evolution,
- Corrections for exact system evolution,
- Populations and averages computations

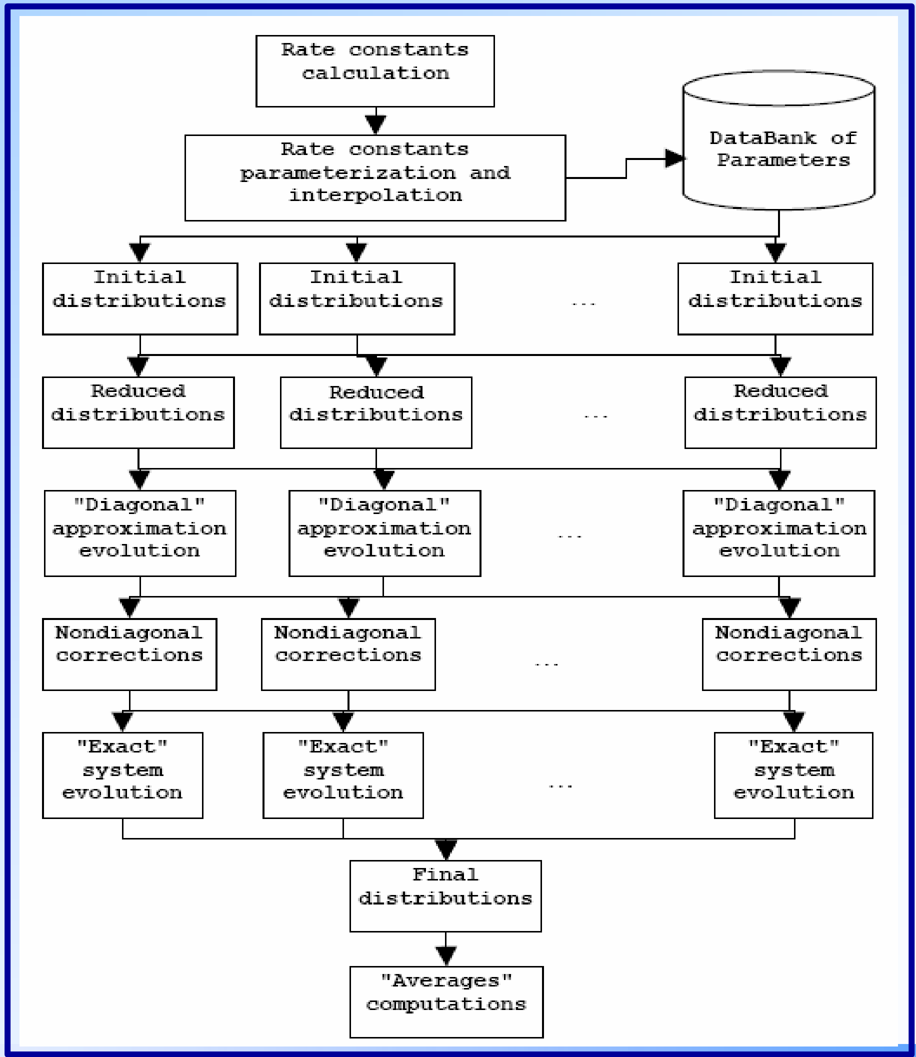
The basic principles of the Grid for kinetics calculation

- 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.

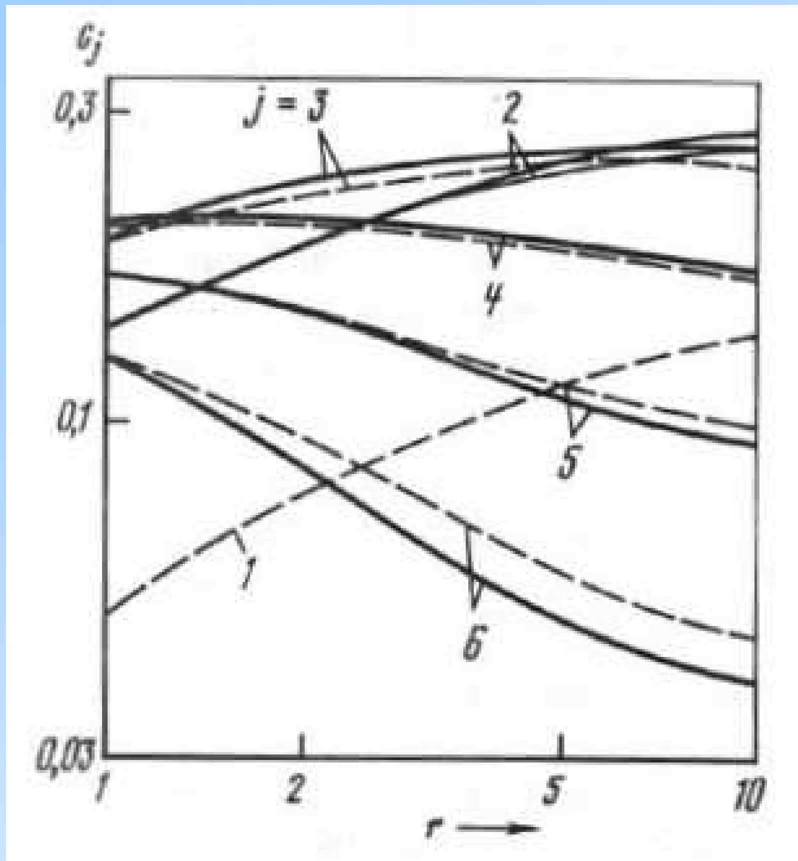
Using Grid for solution of the reactive scattering problem

- 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 approximat
- Computation of exact solution corrections,
- Determination of final distributions,
- Computations of averages,
- Visualization of the results.

The parallel scheme of computing process.

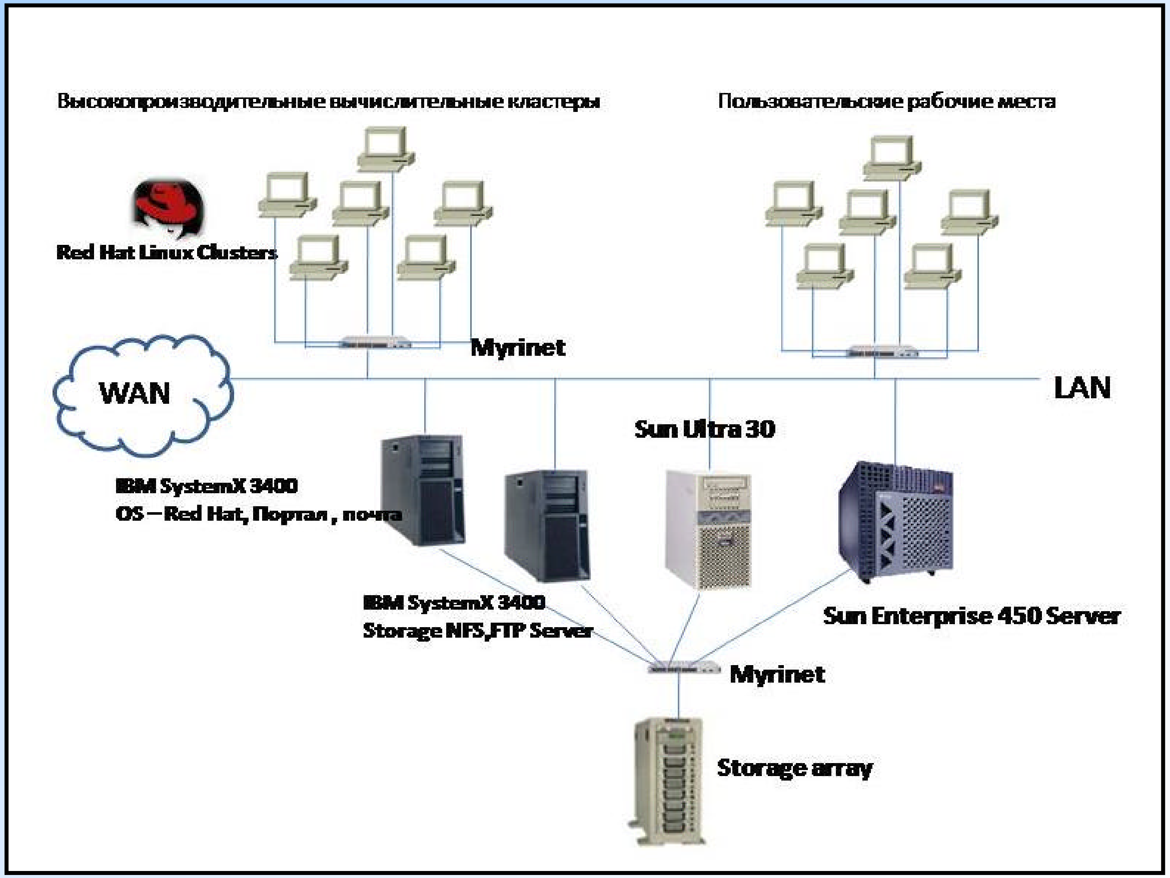


Important Example



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

TESTBED



Высокопроизводительные вычислительные кластеры
Пользовательские рабочие места
Red Hat Linux Clusters
Myrinet
WAN
LAN
Sun Ultra 30
IBM SystemX 3400
OS – Red Hat, Портал , почта
IBM SystemX 3400
Storage NFS,FTP Server
Sun Enterprise 450 Server
Myrinet
Storage array

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