Parallel Integration of Hydrodynamical Approximations of the Boltzmann Equation for rarefied gases on a Cluster of Computers

José Miguel Mantas Ruiz

Software Engineering Department. University of Granada

C/ P. Daniel de Saucedo s/n. 18071 Granada, Spain

e-mail: jmmantas@ugr.es

Phone.: +34 958 243176, Fax: +34 958 243179

Lorenzo Pareschi

Department of Mathematics. University of Ferrara

Via Machiavelli 35, I-44100 Italy

e-mail: pareschi@dm.unife.it

Phone.: +39 0532 974027, Fax: +39 0532 247292

José Antonio Carrillo de la Plata

Department of Applied Mathematics. University of Granada

Avda. Severo Ochoa s/n, 18071 Granada, Spain

e-mail: carrillo@ugr.es

Phone.: +34 958 240827, Fax: +34 958 248596

Julio Ortega Lopera

Computer Architecture and Technology Department. University of Granada.

C/ P. Daniel de Saucedo s/n. 18071 Granada, Spain

e-mail: jortega@atc.ugr.es

Phone.: +34 958 243228, Fax: +34 958 24 89 93

Abstract

The relaxed Burnett system, recently introduced in [5] as hydrodynamical approximation of the Boltzmann equation, is numerically solved. Due to the stiffness of this system and the severe CFL condition for large Mach numbers, a fully implicit Runge-Kutta method has been used. In order to reduce computing time, we apply a parallel stiff ODE solver based on 4-stage Radau IIA IRK. The ODE solver is combined with suitable first order upwind and second order MUSCL relaxation schemes for the spatial derivatives. Speedup results and comparisons to DSMC and Navier-Stokes approximations are reported for a 1D shock profile.

Keywords: Parallel Numerical Algorithms, Boltzmann equation, Burnett equations, Parallel Stiff ODE solvers, relaxation, Implicit Runge-Kutta methods.

2000 MR Subject Classification: 65Y05, 76P05, 65L05, 35L99.

Figure Captions

Figure 1: Speedup results with $P = 4$ and $P = 8$.

Figure 2: Numerical Solution of Navier-Stokes (NS) and Relaxed-Burnett (RB) equations for Mach Number 4 at time t=100.

Figure 3: Numerical Solution of Navier-Stokes (NS) and Relaxed-Burnett (RB) equations for Mach Number 10 at time t=100.

1 Introduction

The Boltzmann equation represents a model for rarefied gas dynamics of monatomic gases or mixtures [1]. Due to the large number of dimensions of the Boltzmann equation (evolution equation in 6 dimensions for a simple monoatomic gas), one has to resort to alternative numerical methods to obtain an approximation to its solution. In real applications, two methods are mainly used: DSMC (Direct Simulation Monte-Carlo) and moment methods. Although DSMC offers less computational cost and greater versatility, it yields low accuracy and statistically fluctuating results, slow convergence and transients are poorly resolved. Since the deterministic solution of the Boltzmann equation is a challenging problem, not only because of the high dimensionality of the equation but also because of the conservation properties of the collision operator, one usually reduces the problem by studying the evolution of certain moments of the density function. Moment methods consist of taking averages of the Boltzmann equation over the velocity variable and make, by some assumption or expansion procedure, a closure to relate higher order moments to low order moments.

Here, we focus on a moment system introduced recently by S. Jin and M. Slemrod [5], called the relaxed Burnett (RB) system. In [4], a numerical scheme for this system based on a semi-implicit discretization of the equation combined with central schemes on staggered grids has been proposed. This scheme gives rather good results in 1D for various Mach numbers in the range $[1, 10]$. However it is observed that for large Mach numbers a severe CFL condition is required. As a consequence, the use of explicit methods to perform the time integration of this system is impractical.

The stiffness and the particular structure of the relaxed Burnett system, demands a great deal of computing power. Here we have modified the spatial discretization of the relaxed Burnett system in 1D, in order to apply a general purpose time integration solver for the stiff ODE's system. Following a component-based methodology to derive parallel ODE solvers, a distributed implementation of a powerful parallel numerical method based on a Radau IIA implicit Runge-Kutta method (IRK) has been obtained. This parallel program is applied to the stiff ODE system resulting as discretization of the RB system (method of lines) and computed on a cluster of PC's.

The parallel stiff ODE solver has been used to solve a test problem of a 1D shock profile. Comparisons with respect to the Navier-Stokes system (NS) and speedup results of the parallel stiff ODE solver with respect to the RADAU5 stiff ODE solver [3] are provided for various Mach numbers and meshes. Our parallel solver is shown to be particularly suited to solve this

problem, since it keeps similar time and spatial accuracy as sequential methods [4] and the computing time is considerably reduced (see Figure 1).

2 The 1D Relaxed Burnett System

The relaxed Burnett system for 1D [5, 4] can be written in the following form:

$$\begin{aligned} U_t + F(U,V)_x &= 0 \\ V_t + G(U,V,U_x,V_x) &= D(U,V,U_x,V_x)_x \end{aligned} \tag{1}$$

where

$$U = \begin{pmatrix} \rho \\ m = \rho u \\ z = \frac{1}{2}\rho u^2 + \frac{3}{2}p \end{pmatrix}, \quad V = \begin{pmatrix} \sigma \\ q \end{pmatrix},$$

$$F(U,V) = \begin{pmatrix} \rho u \\ \rho u^2 + p + \sigma \\ \frac{1}{2}\rho u^3 + \frac{5}{2}up + \sigma u + q \end{pmatrix},$$

$$G(U,V,U_x,V_x) = \begin{pmatrix} u\sigma_x - \frac{4}{3}\sigma u_x + \frac{2p}{\omega_2 \mu}\left(\sigma - \tilde{\sigma}_{eq}\right) \\ uq_x - qu_x + \frac{3\mathcal{M}p}{2\theta_2 \mu}\left(q - \tilde{q}_{eq}\right) \end{pmatrix},$$

$$D(U,V,U_x,V_x)_x = \begin{pmatrix} \frac{p\hat{\omega}_4}{\mu\omega_2}\left[\frac{\mu^3\theta}{\mathcal{M}R\rho^2}\left(\frac{\sigma}{\mu\theta}\right)_x\right]_x \\ \frac{p\hat{\theta}_4}{\mu\theta_2}\left[\frac{\mu^3\theta}{\rho^2}\left(\frac{q}{R\mu\theta^2}\right)_x\right]_x \end{pmatrix},$$

in which the equilibrium values $\tilde{\sigma}_{eq}$, $\tilde{q}_{eq}$ are given by

$$\tilde{\sigma}_{eq} = -\frac{4}{3}\mu u_x + \sigma_2 + \sigma_3,$$

with

$$\begin{aligned} \sigma_2 &= -\mu\frac{\omega_1}{2p}\sigma u_x + \frac{\omega_2 \mu'(\theta)\dot{\theta}}{2p}\sigma - \mu^2\frac{4\omega_3}{9\rho\theta}\left(\frac{q}{\mu\mathcal{M}R}\right)_x \\ &- \mu\frac{4\omega_4}{9\rho p\theta}\frac{q}{\mathcal{M}R}p_x - \mu\frac{4\omega_5}{9\rho\theta^2}\frac{q}{\mathcal{M}R}\theta_x - \mu\frac{\omega_6}{6p}\sigma u_x, \\ \sigma_3 &= \mu^2\left[\frac{2\hat{\omega_2}}{3p^2}{u_x}^2 + \hat{\omega}_3\frac{{\theta_x}^2}{R\rho^2\theta^3}\right]\sigma - \mu\frac{\hat{\gamma_1}}{p\theta}\frac{2}{3\rho R}\left(\sigma^2 u_x + \sigma q_x\right), \\ \dot{\theta} &= \frac{-2}{3\rho R}(pu_x + \sigma u_x + q_x) \end{aligned}$$

and

$$\tilde{q}_{eq} = -\frac{3}{2}\mu\mathcal{M}R\,\theta_x + q_2 + q_3,$$

with

$$
\begin{aligned}
q_2 &= -2\mu\frac{\theta_1}{3\mathcal{M}R\rho\theta}qu_x + \frac{2\theta_2\dot{\theta}\mu'(\theta)}{3\mathcal{M}R\rho\theta}q \\
&\quad -\mu\frac{\theta_3}{2p\rho}\sigma p_x - \mu^2\frac{\theta_4}{2\rho}\left(\frac{\sigma}{\mu}\right)_x - \mu\frac{\theta_5}{2\rho\theta}\sigma\theta_x, \\
q_3 &= \mu^2\left[\frac{2\hat{\theta_2}}{3p^2}{u_x}^2 + \hat{\theta}_3\frac{{\theta_x}^2}{R\rho^2\theta^3}\right]q - \mu\frac{\hat{\lambda_1}}{\rho\theta^2}\frac{2}{3\rho R}\left(\sigma u_x + q_x\right)\left(\frac{q}{\frac{3}{2}\mathcal{M}R}\right).
\end{aligned}
$$

In this system, we have five independent variables ρ (mass density), $m = \rho u$ (momentum, where u is the macroscopic velocity), $z = \frac{1}{2}\rho u^2 + \frac{3}{2}p$ (total energy, where p is the normal pressure), σ (pressure deviation tensor) and q (heat flux vector). Here θ is the temperature, μ is the viscosity ($\mu = \mu(\theta)$), $\mathcal{M}$ is the Maxwell number ($\mathcal{M} \simeq \frac{5}{2}$) and R is the perfect gas constant.

The symbols $\omega_1, \ldots, \omega_6, \theta_1, \ldots, \theta_5, \hat{\omega}_2 \ldots, \hat{\omega}_4, \hat{\theta}_2, \ldots \hat{\theta}_4, \hat{\gamma_1}$ and $\hat{\lambda_1}$ denote coefficients of the relaxed Burnett system. The approximated values for these constants are given by [4]

$$
\begin{gathered}
\omega_1 = \frac{10}{3}, \quad \omega_2 = 2, \quad \omega_3 = 3, \quad \omega_4 = 0, \quad \omega_5 = 3, \quad \omega_6 = 8, \\
\theta_1 = \frac{225}{24}, \quad \theta_2 = \frac{45}{8}, \quad \theta_3 = -3, \quad \theta_4 = 3, \quad \theta_5 = \frac{117}{4}, \qquad \hat{\gamma_1} = 0, \quad \hat{\lambda_1} = \frac{-45}{16} \\
\hat{\omega}_2 = \hat{\omega}_3 = \hat{\omega}_4 = 20, \qquad \hat{\theta}_2 = -60, \quad \hat{\theta}_3 = 100, \quad \hat{\theta}_4 = 25.
\end{gathered} \tag{2}
$$

The values of the parameters $\hat{\omega}_i$ and $\hat{\theta}_i$, $i = 1, \ldots, 4$ have been computed by a least square fitting with DSMC results for Mach 4 [4].

3 Spatial Discretization

We have obtained a stiff ODE system from the spatial discretization of the RB system for 1D. The infinite physical space is truncated to the finite region $[0, L]$ where L depends on the Mach number considered. We have subdivided this interval into $N-1$ intervals of length $\Delta x = \frac{L}{N-1}$.

To obtain the spatial discretization of $F(U,V)_x$, we have applied the relaxation approximation presented in [6]. Precisely, we have studied the application of two relaxation schemes in the zero relaxation limit [6]. First we have splitted $F(U,V)_x = F^1(U)_x + F^2(U,V)_x$. In the sequel we noted $F = F^1$ for simplicity.

- **First-order upwind relaxation scheme**

  An approximation of $U_t + F(U)_x = 0$, gives:

$$
\frac{\partial}{\partial t}U_j = -\frac{1}{2\Delta x}\Big(F(U_{j+1}) - F(U_{j-1}) + A^{1/2}(U_{j+1} - 2U_j + U_{j-1})\Big) = [F(U)_x]_j^{upwind},
$$

Here, $U_j, \quad j = 1, ..., N$, is the approximation to the vector U at the j-th grid point. The matrix A is a diagonal matrix of positive values $a_i, \quad i = 1, ..., 3$ which are selected in order to ensure the dissipative nature of the system [6].

- **Second-order MUSCL relaxation scheme**

  In this case, the spatial discretization is a perturbation of the first order upwind, namely:

$$\frac{\partial}{\partial t}U_j = [F(U)_x]_j^{upwind} + \frac{1}{4}(s_{j+1}^- - s_j^+ - s_j^- + s_{j-1}^+) = [F(U)_x]_j^{MUSCL}, \qquad j = 1, ..., N.$$

  Here, $s_j^{\pm}$ is the slope of $F(U_j) \pm A^{1/2}U_j$ [6].

These are consistent and stable discretizations of $F(U)_x$. The splitting of $F(U, V)$ into $F^1(U) + F^2(U, V)$ allows us to use the same relaxation matrix A as for the Euler system [6].

We have discretized the spatial derivatives in $F^2(U, V)_x$, $G(U, V, U_x, V_x)$ and $D(U, V, U_x, V_x)_x$ in the RB equations for the stress deviator and heat flux (which are not in conservative form), by using second-order central finite differences. This spatial discretization on the grid $(x_1, x_2, \ldots, x_N)$ leads to a system of $5N$ differential equations. These equations have been ordered according to

$$\begin{array}{ccccc} (\rho_t)_{x=x_1}, & (m_t)_{x=x_1}, & (z_t)_{x=x_1}, & (\sigma_t)_{x=x_1}, & (q_t)_{x=x_1}, \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (\rho_t)_{x=x_N}, & (m_t)_{x=x_N}, & (z_t)_{x=x_N}, & (\sigma_t)_{x=x_N}, & (q_t)_{x=x_N}. \end{array}$$

With this ordering, the ODE system has a banded structure with 9 subdiagonals and 7 superdiagonals. This structure will have to be taken into account in order to perform efficiently the time integration.

4 A Parallel Stiff ODE solver to Perform the Time Integration

The ODE system which arises from the spatial discretization of the relaxed Burnett system contains stiff terms because it has been obtained by applying a relaxation scheme [6] and a severe CFL condition is required for large Mach numbers. Therefore, an implicit method must be used to perform the time integration. Since the resulting system is nonlinear, solving the time discretization is highly expansive and it may benefit from the use of parallel processing.

We start from an efficient and powerful parallel numerical scheme to solve stiff ODEs [10, 7]. This scheme is based on a Radau IIA implicit Runge-Kutta method with 4 stages [3]

and exhibits excellent convergence and stability properties. The parallel numerical scheme is a mixture of direct and iterative algorithms to solve the nonlinear systems which arise when the Radau IIA method [3] with 4 stages is applied. As a result, the computation of each stage of the method can be performed in parallel. Additionally, this method has been optimized in [8] by reducing computation costs and increasing the task parallelism. In order to select dynamically the stepsize through the time integration, the scheme uses a strategy which is very similar to that used in the RADAU5 solver [3].

An efficient implementation of this numerical scheme for a cluster of Personal Computers has been developed. For that, we have applied a component-based methodology to derive parallel ODE solvers [9, 8]. This methodology allows the exploitation of the task and data parallelism of the numerical scheme and the structure of the problem to be solved, in order to minimize the execution time.

Following this methodology, the parallel numerical scheme has been efficiently implemented on a cluster of PCs based on Pentium II. We have obtained two versions of this solver, one optimized for 4 processors and another optimized for 8 processors.

The implementation uses the parallel routines of LAPACK and ScaLAPACK libraries [2] to take advantage of the potential parallelism of the scheme and the banded structure of the ODE system. The parallelism inherent in the ODE system and the structure is also exploited by using a parallel block routine for the evaluation of the ODE system. The remote communication which is required to obtain local portions of the subvectors in each processor is reduced substantially taking into account the banded structure of the ODE system. This structure is also taken into account to reduce the cost in the computation of the Jacobian matrix. The structure of the system is also used at each stage and step of the iterative method by particular library routines for banded matrices.

5 Experimental Results

The relaxation model has been considered in the form (1) with $\mu = \epsilon\theta$ (ϵ is the Knudsen number), $R = 1$ and the set of parameters given by (2).

The test problem is given by a one-dimensional stationary shock profile for $\epsilon = 1$ and different values of the Mach number ranging from 1.4 to 10. In all our numerical examples the gas is initially at the upstream equilibrium state in the left half-space and in the downstream equilibrium state in the right-half space. The two states being smoothly connected with an hyperbolic tangent function. We compare our results to the reference solution given by the

DSMC method.

The parallel code is applied to solve the test problem. We report the result obtained with the Navier-Stokes equations and the Burnett relaxed system, using several space cell numbers at time $t = 100$ after the stationary state has been reached. The NS system is obtained as a particular case of our RB system by taking the σ and q variables to the following values:

$$\sigma = -\frac{4}{3}\mu u_x, \qquad q = -\frac{3}{2}\mu \mathcal{M} R\, \theta_x.$$

We omit the results obtained with Mach number 1.4 because the results obtained by integrating NS and RB equations are very similar and they provide a reasonable good description of the rarefied shock.

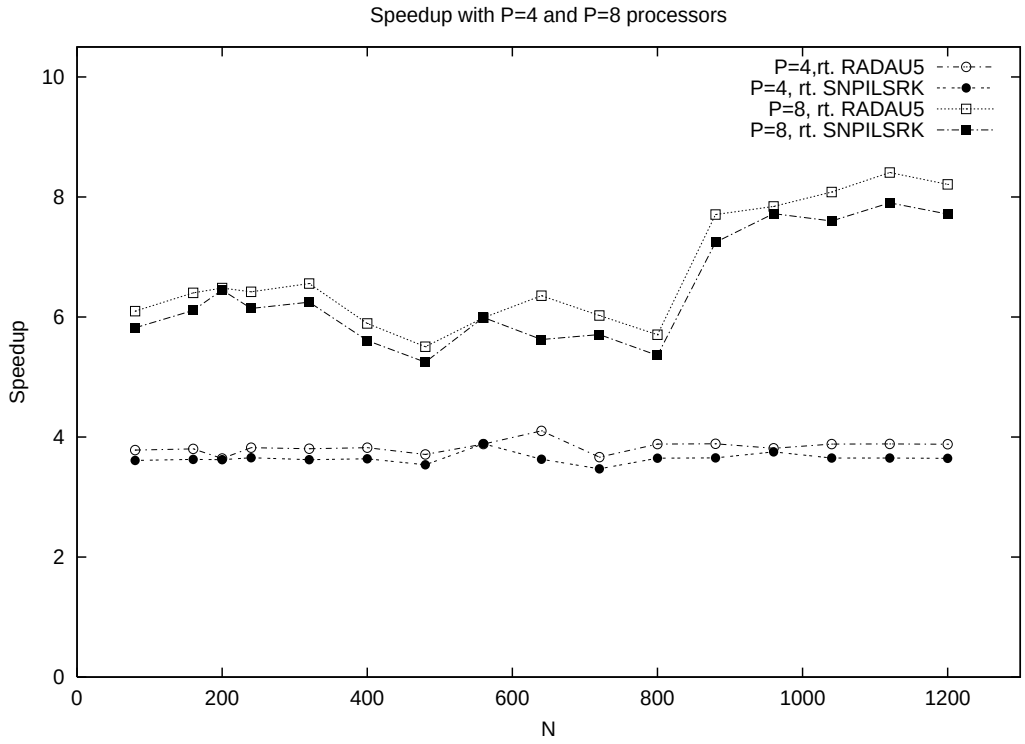
The results with Mach number 4, $t = 100$, and 800 grid points is shown in figure 2. In this figure, the solutions obtained by integrating the NS and RB equations, for the density $\rho(x,t)$, the velocity $u(x,t)$, the temperature $\theta(x,t)$, $\sigma(x,t)$) and $q(x,t)$, are compared to the reference solution given by the DSMC method.

We also compare the results obtained by the upwind relaxed scheme with a fine grid ($N = 800$ points), with the results obtained by the MUSCL relaxed scheme with a coarse grid ($N = 200$ points). The numerical experiments show that the results are very similar in both cases (upwind with 800 points and MUSCL with 200 points) and a marked improvement of the numerical solution with respect to NS model is achieved in both cases. Despite of the advantage of using less grid points, the use of the MUSCL scheme in the spatial discretization requires very small stepsize (330 time steps for the upwind scheme and more than 4000 steps for the MUSCL to achieve the same final time) and the computational cost of each integration step is greater. The use of MUSCL instead of the upwind scheme might only be justified if one is interested in computing discontinuous shock profiles or when there are strong constrainsts in the storage available for the computational system.

With Mach Number $M = 10.0$ (see figure 3), we only show the results of the RB model when the upwind scheme is used in the spatial discretization because of previous reasons. The numerical results obtained for the RB model represent a marked improvement with respect to the NS model. Finally, we want to remark that the computation for larger Mach numbers (> 10) with this approach has not been possible yet. The main difficulty is to find stable approximations of the nonconservative system (1). These issues are currently under investigation.

In order to show the benefits of performing the time integration in parallel, we have calculated the speedups of our parallel solver by considering two sequential stiff ODE solvers:

Figure 1:



- one of the most robust and efficient sequential stiff ODE solvers, the experimental code *RADAU5* [3], based on a Radau IIA method with 3 stages (order 5),
- a sequential implementation of the optimized Newton-PILSRK (Parallel Iterative Linear System Solver for Runge-Kutta) method that we called SNPILSRK [10, 8].

Both sequential solvers take advantage of the banded structure of the ODE system.

We report the parallel speedup results obtained on 4 and 8 processors (see figure 1). These results have been obtained by comparing the parallel execution times for $P = 4$ and $P = 8$ processors, with the execution time of the sequential programs (SNPILSRK and RADAU5) running on a single processor of the PC cluster. The time results were taken on an integration step, starting from the initial state, for Mach Number 10 and meshes varying form $N = 80$ to $N = 1200$.

The experiments reveal that a speedup of 3.2 to 3.85 can be achieved on 4 nodes and a speedup of 5.2 to 7.9 can be achieved on 8 nodes with regard to the SNPILSRK solver. The speedup values obtained with respect to RADAU5 solver are only a slight improvement. Our SNPILSRK solver is slightly faster than the sequential version of RADAU5 as seen in Figure 1, where speedups with respect to the parallel solver are slightly higher for RADAU5 than those obtained by using SNPILSRK.

Acknowledgements

The experimental results of this work were obtained on a PC cluster supported by the project TIC97-1149 of the CICYT. The first three authors acknowledge partial support of a bilateral Italian-Spanish program HI2001-0175.

References

[1] C. Cercignani, R. Illner, and M. Pulvirenti. *The Mathematical Theory of Diluted Gases.* Springer-Verlag, 1994.

[2] J. J. Dongarra and D. W. Walker. *Software libraries for linear Algebra Computations on High Performance Computers.* SIAM Review, 1995.

[3] E. Hairer and G. Wanner. *Solving Ordinary Differential Equations II: Stiff and Differential Algebraic Problems.* Springer-Verlag, 1996.

[4] Shi Jin, Lorenzo Pareschi, and Marshall Slemrod. *A Relaxation Scheme for Solving the Boltzmann Equation Based on the Chapman-Enskog Expansion.* Acta Mathematicas Applicatae Sinica (English Series), 18, 2002.

[5] Shi Jin and Marshall Slemrod. *Regularization of the Burnett equations via relaxation.* J. Stat. Phys., 103, 5-6, 2001.

[6] Shi Jin and Zhouping P. Xin. *The Relaxation Schemes for Systems of Conservation Laws in Arbitrary Space Dimensions.* Communication on Pure and Applied Mathematics, 48:235–276, 1995.

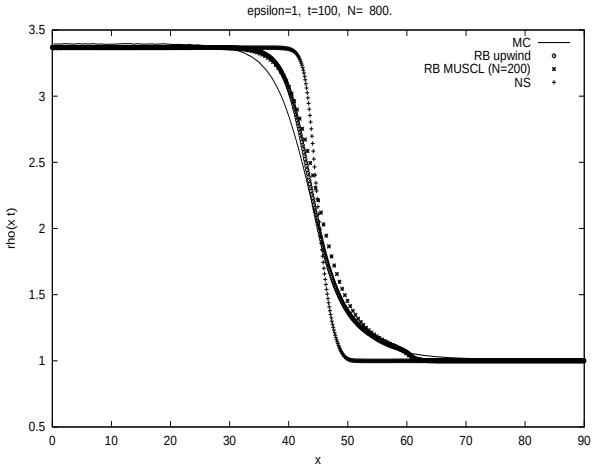
[7] J. M. Mantas and J. Ortega Lopera. *A Component-Based Stiff ODE Solver on a Cluster of Computers.* 4th International Meeting on Vector and Parallel Processing, VECPAR'2000, Jun. 2000.

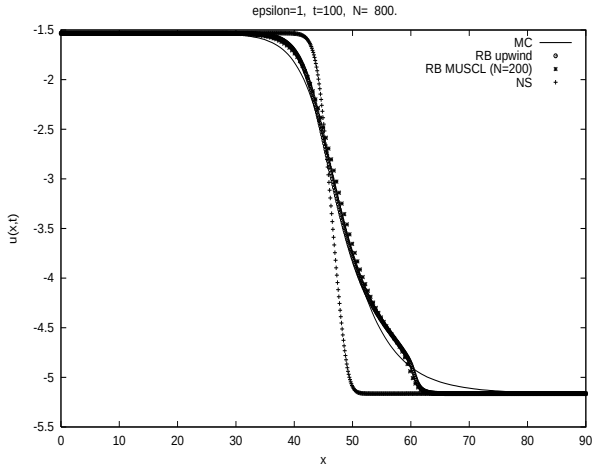
[8] J. M. Mantas, J. Ortega Lopera, and J. A. Carrillo. *Component-Based Derivation of a Stiff ODE Solver implemented on a PC Cluster.* International Journal of Parallel Programming, 30(2), Apr. 2002.

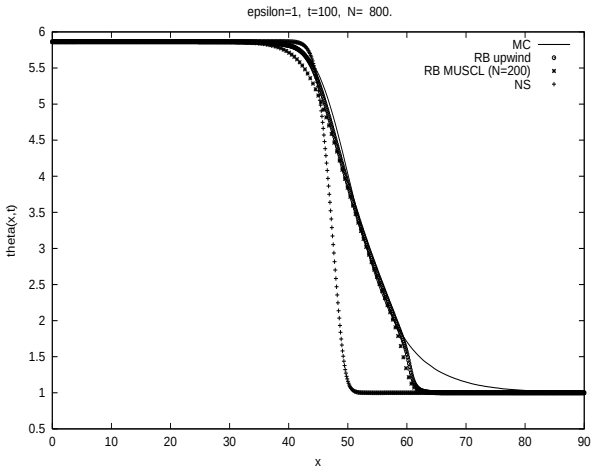
[9] J. M. Mantas, J. Ortega Lopera, and J. A. Carrillo. *Exploiting the Multilevel Parallelism and the Problem Structure in the Numerical Solution of Stiff ODEs.* 10th Euromicro Workshop on Parallel, Distributed and Network-based Processing, 2002.

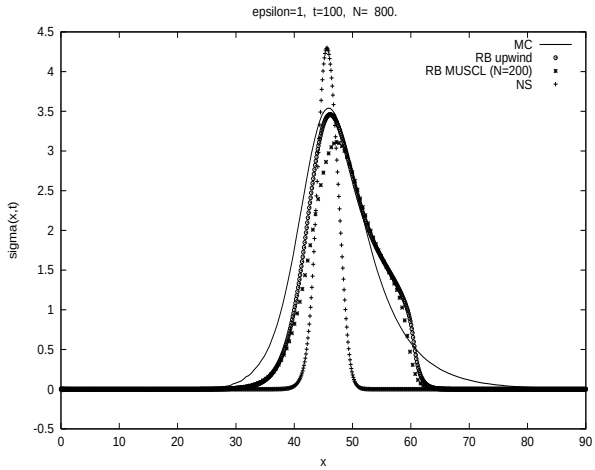
[10] P. J. Van der Houwen and J. J. B. de Swart. *Parallel linear system solvers for Runge-Kutta methods.* Advances in Computational Mathematics, 7:157–181, Mar. 1997.

Figure 2:


epsilon=1, t=100, N= 800.
MC
RB upwind
RB MUSCL (N=200)
NS
rho(x,t)
x


epsilon=1, t=100, N= 800.
MC
RB upwind
RB MUSCL (N=200)
NS
u(x,t)
x


epsilon=1, t=100, N= 800.
MC
RB upwind
RB MUSCL (N=200)
NS
theta(x,t)
x


epsilon=1, t=100, N= 800.
MC
RB upwind
RB MUSCL (N=200)
NS
sigma(x,t)
x

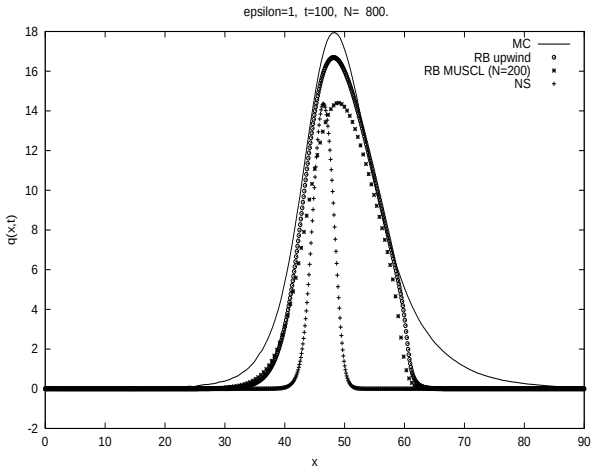
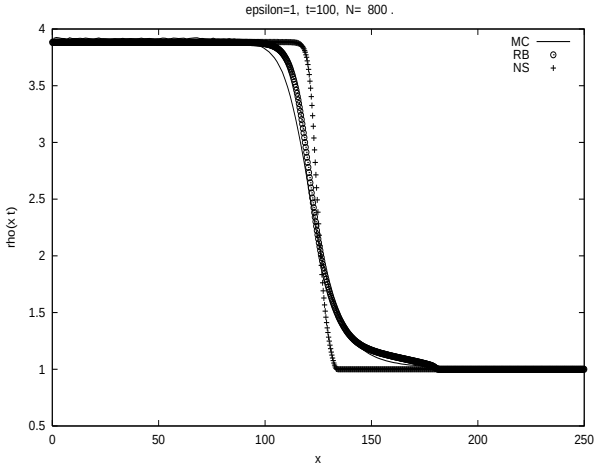
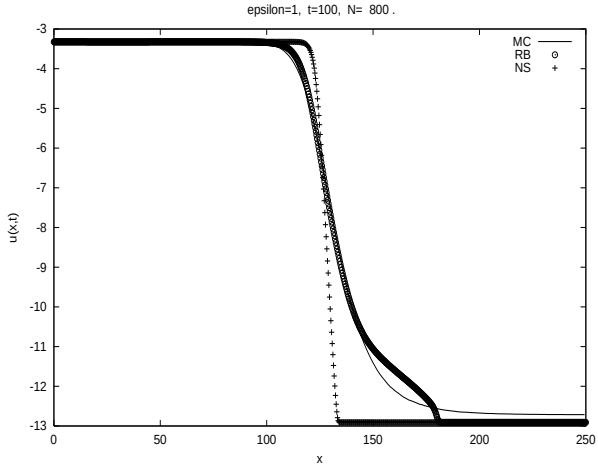
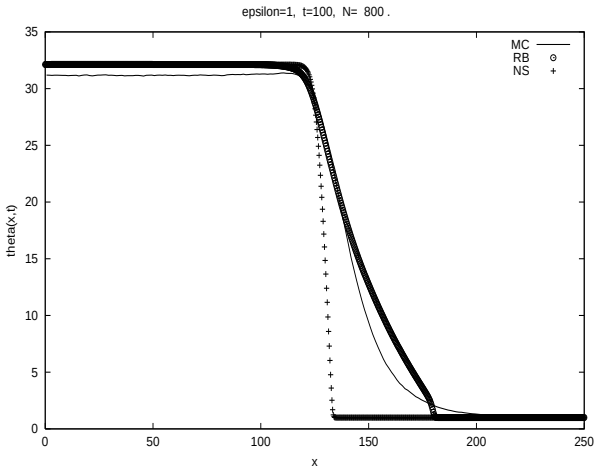
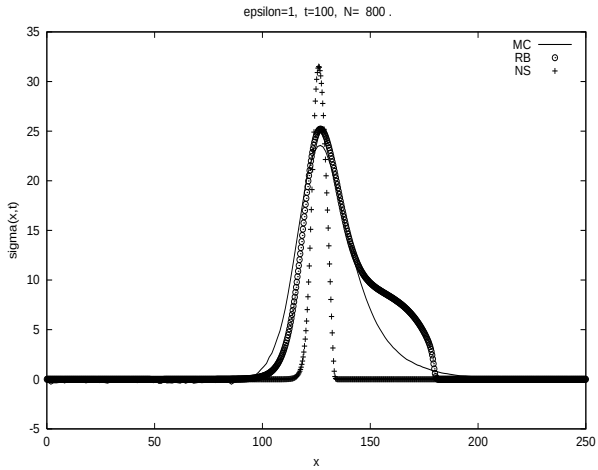

epsilon=1, t=100, N= 800.
MC
RB upwind
RB MUSCL (N=200)
NS
q(x,t)
x

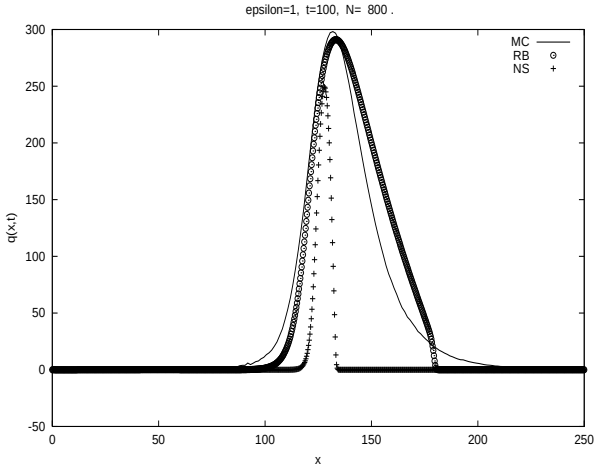
Figure 3:


epsilon=1, t=100, N= 800 .
MC
RB
NS
rho(x,t)
x


epsilon=1, t=100, N= 800 .
MC
RB
NS
u(x,t)
x


epsilon=1, t=100, N= 800 .
MC
RB
NS
theta(x,t)
x


epsilon=1, t=100, N= 800 .
MC
RB
NS
sigma(x,t)
x


epsilon=1, t=100, N= 800 .
MC
RB
NS
q(x,t)
x