Analysis of over-relaxation kinetic schemes: application to the development of stable and second order boundary conditions.

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**CONTEXT**

### Equations to be solved numerically

- systems of conservation laws:
  \[ \partial_t W + \text{div} \left( F(W) \right) - \text{div} \left( D(x, W) \nabla W \right) = S \]

- example: the ideal MHD equations
  \[
  \begin{align*}
  \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) &= 0 \\
  \rho \partial_t \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - (\nabla \times \mathbf{B}) \times \mathbf{B} &= 0 \\
  \partial_t p + \nabla \cdot (\rho \mathbf{u}) + (\gamma - 1) \rho \nabla \cdot \mathbf{u} &= 0 \\
  \partial_t \mathbf{B} - \nabla \times (\mathbf{u} \times \mathbf{B}) &= 0 \\
  \nabla \cdot \mathbf{B} &= 0
  \end{align*}
  \]

### Challenges

Two characteristics:
1. nonlinear systems of equations,
2. waves associated with different time scales \( \Rightarrow \) we want to resolve only some of these scales.

Numerically they imply that:
- **explicit schemes** have very restrictive CFL conditions, due to the fastest time scales,
- **implicit schemes** involve nonlinear operator inversion, expensive matrices storage and inversions.
**Lattice-Boltzmann and Vectorial Schemes**

Equations to be solved numerically

\[ \partial_t W + \text{div} \left( F(W) \right) - \text{div} \left( D(x, W) \nabla W \right) = S \]

**Lattice-Boltzmann methods**

- inspired from the kinetic theory,
- discrete set of velocities: choice of a Lattice (ex: D2Q9)

\[ \begin{align*}
&v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8, v_9, v_{10} \\
&0
\end{align*} \]

- collision step: \( f_i(t, x) = f_i^{eq}(t, x) \)
- shift step: \( f_i(t + \Delta t, x) = f_i(t, x - v_i \Delta t) \)
- macroscopic variables: \( \rho = \sum_i f_i, \quad \rho u = \sum_i v_i f_i, \quad E = \sum_i |v_i|^2 / 2f_i \)
- Navier-Stokes equations,
- equivalent kinetic equation with BGK collision operator (LBGK scheme):

\[ \partial_t f_i + v_i \cdot \nabla f_i = \epsilon_i^{-1} \left( f_i^{eq} - f_i \right) \]

**Vectorial kinetic schemes**

- generalization of Jin-Xin relaxation scheme, [Jin and Xin, 1995]

\[ \begin{align*}
\partial_t W + \partial_x Z &= 0 \\
\partial_t Z + \lambda^2 \partial_x W &= \epsilon^{-1} (F(W) - Z)
\end{align*} \]

- ex: D2Q4 scheme:

\[ \begin{align*}
v_1, v_2, v_3, v_0
\end{align*} \]

- kinetic equations with relaxation source term:

\[ \partial_t f_i + v_i \cdot \nabla f_i = \epsilon_i^{-1} (f_i^{eq} - f_i) \]

- macroscopic variables: \( \rho = \sum_i f_i, \quad \rho u = \sum_i g_i, \quad \rho v = \sum_i h_i \ldots \)
AN EXAMPLE OF LBGK CODE

Vectorial kinetic systems

\[ \partial_t f + \Lambda \nabla f = \frac{f^{eq} - f}{\epsilon} \]

Ideas in the kirsch code [Coulette et al., 2018]

► Time integration:
  • time splitting approach,
  • second-order Crank-Nicolson integration for both steps
    ⇒ implicit relation between \( f_{i,j}^{n+1} \) and \( f_{i,j}^n \), ⇒ large time steps,
  • higher time order thanks to composition methods, [Suzuki, 1990]

► transport step: high-order DG on H2O grids,

► two levels of parallelism:

1 parallelization over the kinetic velocities,

2 grid decomposition into macrocells and cartesian sub-grids:
  • the linear system is block-triangular,
  • inversion of matrices in sub-grids (using KLU),
  • graph of macro-cells resolution:

\[
f_{i,j}^{n+1} = \frac{\theta \alpha_i}{1 + \theta \alpha_i} f_{i,j}^{n+1} + \frac{1 - (1 - \theta) \alpha_i}{1 + \theta \alpha_i} f_{i,j}^n + \frac{(1 - \theta) \alpha_i}{1 + \theta \alpha_i} f_{i,j}^n - 1
\]

► task-scheduling programming (StarPU).
ISSUE OF THE BOUNDARY CONDITIONS

One of the current issues of the LBM approach is the treatment of the boundary conditions:

▶ **ex:** nD2Q4 scheme,
▶ here \( f_1 \) and \( f_3 \) are outgoing quantities
  ⇒ no problem,
▶ \( f_0 \) and \( f_2 \) are incoming quantities
  ⇒ what are their values?
▶ the macroscopic equation provides only one boundary condition,

⇒ **one relation is missing!**

Objectives of this work

▶ Study of the second order over-relaxation scheme used to solve nD1Q2 relaxation systems,
▶ design boundary conditions that preserve the scheme second order.
## CONTENTS OF THE PRESENTATION

**Relaxation schemes:**
- the Jin-Xin relaxation model,
- relation with the vectorial kinetic schemes,
- splitting and composition strategies,
- an example of MHD code.

**The over-relaxation scheme:**
- derivation from the standard relaxation approach,
- equivalent equation and properties of the over-relaxation scheme,
- stability condition for the 1D transport equation.

**Boundary conditions:**
- usual boundary conditions for LBM,
- inflow/outflow conditions,
- numerical results.
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# THE JIN-XIN RELAXATION SCHEME

## Equations to be solved (1D)

\[
\partial_t V + \partial_x F(V) = 0
\]  
(1)

**recall:** nonlinear flux functions \( V \mapsto F(V) \).

## The relaxation model

- approximate systems (1) by systems of linear-flux equations:
  \[
  \begin{align*}
  \partial_t W_\epsilon + \partial_x Z_\epsilon &= 0, \\
  \partial_t Z_\epsilon + \lambda^2 \partial_x W_\epsilon &= \frac{1}{\epsilon} (F(W_\epsilon) - Z_\epsilon),
  \end{align*}
  \]  
(2) \hspace{5cm} (3)

- a Chapman-Enskog development gives:
  
  - at zeroth order in \( \epsilon \):
    \[
    Z_\epsilon = F(W_\epsilon) + O(\epsilon),
    \]
  
  - at first order in \( \epsilon \):
  
    \[
    \partial_t W_\epsilon + \partial_x F(W_\epsilon) = \epsilon \partial_x \left( \left( \lambda^2 - \left| \partial F(W_\epsilon) \right|^2 \right) \partial_x W_\epsilon \right) + O(\epsilon^2)
    \]  
(4)

- **consistency** of equation (4) with equation (1),

- **stability** under the subcharacteristic condition: \( \lambda > |\partial F(W_\epsilon)| \).

## Numerical scheme

Numerical resolution of system (2)-(3) in the \( \epsilon = 0 \) limit.
**VECTORIAL KINETIC SCHEMES**

### From Jin-Xin to D1Q2 system

- **Jin-Xin relaxation model:**
  \[
  \frac{\partial W}{\partial t} + \frac{\partial Z}{\partial x} = 0, \\
  \frac{\partial Z}{\partial t} + \lambda^2 \frac{\partial W}{\partial x} = \varepsilon^{-1} (F(W) - Z),
  \]

- **Riemann invariants:**
  \[
  f^+ = W + \frac{Z}{\lambda}, \quad f^- = W - \frac{Z}{\lambda}
  \]

- **System for the Riemann invariants (nD1Q2):**
  \[
  \frac{\partial f^+}{\partial t} + \lambda \frac{\partial f^+}{\partial x} = \varepsilon^{-1} (f^{eq^+} - f^+), \\
  \frac{\partial f^-}{\partial t} - \lambda \frac{\partial f^-}{\partial x} = \varepsilon^{-1} (f^{eq^-} - f^-),
  \]

- **Equilibrium functions:**
  \[
  f^{eq^+} = W + F(W)/\lambda, \quad f^{eq^-} = W - F(W)/\lambda
  \]

### 2D and 3D systems

- **Kinetic relaxation systems:**
  \[
  \frac{\partial f}{\partial t} + \Lambda \nabla f = \frac{1}{\varepsilon} \left( f^{eq}(W) - f \right), \\
  Pf = W.
  \]

- **Example:**
  D2Q4 system

- **Consistency conditions:**
  \[
  Pf^{eq}(W) = W, \\
  P\Lambda f^{eq}(W) = F(W).
  \]

- **Example:***
  \[
  \Lambda = \text{diag} \{ (\lambda, 0), (\lambda, 0), \}
  \]
  \[
  (0, \lambda), (0, -\lambda) \}, \\
  P = (1, 1, 1, 1).
  \]
**SPLITTING APPROACH AND TIME INTEGRATION (1)**

### Kinetic system to be solved

\[ \partial_t f + \Lambda \nabla f = \frac{1}{\varepsilon} (f^{eq}(W) - f), \]

### Operator splitting

- **Transport step:**
  \[ \partial_t f + \Lambda \nabla f = 0, \]  
  \[ \partial_t f = \frac{1}{\varepsilon} (f^{eq}(W) - f), \]

- **Relaxation step:**

### Transport step over time step \( h: T(h) \)

Possible numerical schemes:

- exact transport on cartesian grid:
  \[ f_i(t+h, x) = f_i(t, x - v_i h), \]
  \[ \Rightarrow \ h \text{ must be compatible with the grid}, \]

- Semi-Lagrangian schemes:
  \[ f_i(t+h, x) = f_i(t, x - v_i h) \]
  \[ \Rightarrow \text{backward SL: interpolation at the foot of the characteristics,} \]
  \[ \Rightarrow \text{forward SL: projection on the mesh,} \]

- high-order FV or DG schemes,
  \[ \Rightarrow \text{implicit schemes require matrix inversion.} \]

### Source integration: \( R(h) \)

Possible integrations over time step \( h: \)

- exact solution of (6), with \( \varepsilon > 0: \)
  \[ f(t+h, x) = f^{eq} + \exp(-h/\varepsilon)(f(t, x) - f^{eq}), \]
  \[ \Rightarrow f^{eq} \text{ is invariant during the integration}, \]

- projection on the equilibrium \( (\varepsilon = 0): \)
  \[ f(t+h, x) = f^{eq}(t, x), \]
  \[ \Rightarrow \text{provides first-order approximation with} \]
  \[ \text{the splitting approach,} \]

- Crank-Nicolson integration:
  \[ f(t+h, x) = (1 - \theta)f^{eq}(t, x) + \theta f(t, x) \]
  with \( \theta = (2\varepsilon - h)/(2\varepsilon + h), \)
  \[ \Rightarrow \text{second-order when} \varepsilon = 0. \]
**SPLITTING APPROACH AND TIME INTEGRATION (2)**

### Kinetic system to be solved

\[ \partial_t f + \nabla \cdot f = \frac{1}{\varepsilon} (f_{eq}(W) - f) , \]

### Lie and Strang splitting

**Lie splitting:**  
\[ L(h) = T(h)R(h) \]  
- first-order splitting

**Strang splitting:**  
\[ S(h) = T(h/2)R(h)T(h/2) \]  
- second-order splitting with Crank-Nicolson,
- higher-order composition not possible...

### Time-symmetry property

Let \( P(h) \) be a discrete operator, dependent on time step \( h \),

- **definition of time symmetry:** \( P(-h)P(h) = I \) and \( P(0) = I \),
- **property:** if \( P(h) \) is consistent with a continuous operator \( P \), then it is a second-order consistency,
  
  [Hairer et al., 2006, McLachlan and Quispel, 2002]
- \( S(h) \) is not time symmetric when \( \varepsilon = 0 \): \( S(0) \neq I \).

### Time composition schemes

From a second-order time-symmetric operator \( P(h) \), one can build even high-order operators with palindromic composition \( Q(h) \):

\[ Q(h) = P(\gamma_0 h)P(\gamma_1 h)\ldots P(\gamma_s h) \]

with \( \gamma_i = \gamma_{s-i}, 0 \leq i \leq s \). **Examples** in: [Suzuki, 1990, Kahan and Li, 1997].
## Example of an MHD Code

### Features of Patapon

- solves the ideal MHD equations,
- nD2Q4 approximation,
- time-symmetric composition with:
  - exact transport step,
  - Crank-Nicolson source integration with $\theta = 0.9$,  
  $\Rightarrow$ numerical resistivity.
- cartesian grid and periodic or Dirichlet BC,
- Python code using PyOpenCL kernels.

### Example of simulation: tilt instability

### Computation characteristics

- 1024 × 1024 grid,
- graphic card: Nvidia - 24 GB - 3840 cores
- GPU utilization: 80%
- computation time: 30s (including I/O)

### Simulation results

![Simulation result]

Time: 6.99 s
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DERIVATION OF THE OVER-RELAXATION SCHEME

System to be solved

\[ \partial_t \mathbf{v} + \partial_x F(\mathbf{v}) = 0 \]  

▶ Two auxiliary sets of variables: \( \mathbf{w}, \mathbf{z} \),
▶ could be considered as relaxation approach with \( \varepsilon = 0 \).

Transport step

\[ \begin{align*}
\partial_t \mathbf{w} + \partial_x \mathbf{z} &= 0, \\
\partial_t \mathbf{z} + \lambda^2 \partial_x \mathbf{w} &= 0,
\end{align*} \]

⇒ exact transport operator:

\[ \left( \begin{array}{c}
\mathbf{w}(\cdot, t + h) \\
\mathbf{z}(\cdot, t + h)
\end{array} \right) = T(h) \left( \begin{array}{c}
\mathbf{w}(\cdot, t) \\
\mathbf{z}(\cdot, t)
\end{array} \right), \]

with

\[ T(h) := \frac{1}{2} \begin{pmatrix}
\tau(h) + \tau(-h) & \lambda(\tau(h) - \tau(-h)) / \lambda \\
\lambda(\tau(h) - \tau(-h)) & \tau(h) + \tau(-h)
\end{pmatrix}, \]

and shift operator

\[ (\tau(h)\mathbf{v})(x) = \mathbf{v}(x - \lambda h). \]

Over-relaxation step

▶ Crank-Nicolson \( (\varepsilon = 0) \):

\[ R_0(h) \left( \begin{array}{c}
\mathbf{w} \\
\mathbf{z}
\end{array} \right) = \left( \begin{array}{c}
\mathbf{w} \\
2F(\mathbf{w}) - \mathbf{z}
\end{array} \right) \]

▶ independent of \( h : R_0 \).

Operator splitting

\[ S_2(h) := T\left( \frac{h}{4} \right) R_0 T\left( \frac{h}{2} \right) R_0 T\left( \frac{h}{4} \right) \]
Equivalent Equation and Scheme Properties

Over-relaxation scheme

\[ S_2(h) := T\left(\frac{h}{4}\right) R_0 T\left(\frac{h}{2}\right) R_0 T\left(\frac{h}{4}\right). \]  (8)

Time-symmetric property

- \( T(-h)T(h) = I \) and \( T(0) = I \)
- \( R_0 R_0 = I \)

\[ \Rightarrow S_2(-h)S_2(h) = I \] and \( S_2(0) = I \).

We expect a second-order scheme.

Example: scalar transport equation:

Example: Euler equations:

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**Theorem 1** [Drui et al., 2018]

\( w \) and \( z \) being smooth solutions of a time marching algorithm with operator (8), the flux error \( y \) being defined by

\[ y := z - F(w), \]

then, up to second order terms in \( h \), \( w \) and \( y \) satisfy:

\[ \partial_t \begin{pmatrix} w \\ y \end{pmatrix} + \begin{pmatrix} F'(w) & 0 \\ 0 & -F'(w) \end{pmatrix} \partial_x \begin{pmatrix} w \\ y \end{pmatrix} = 0. \]
STABILITY FOR THE 1D TRANSPORT EQUATION (THEOREM 2)

1D scalar transport equation

\[ \partial_t u + c \partial_x u = 0 \]

Equivalent equation

\[ \partial_t \left( \begin{array}{c} w \\ y \end{array} \right) + \left( \begin{array}{cc} c & 0 \\ 0 & -c \end{array} \right) \partial_x \left( \begin{array}{c} w \\ y \end{array} \right) + A \Delta t^2 \partial_{xxx} \left( \begin{array}{c} w \\ y \end{array} \right) = O(\Delta t^3), \] (9)

with

\[ A = \left( \begin{array}{cc} (\lambda^2 - c^2) & 3c \\ 3c(\lambda^2 - c^2) & -(\lambda^2 - c^2) \end{array} \right). \]

Conservation of a convex energy

\[ E(t) = \int_{\Omega} \left( (\lambda^2 - c^2) \frac{w^2}{2} + \frac{y^2}{2} \right) = \int_{\Omega} \left( D \left( \begin{array}{c} w \\ y \end{array} \right), \left( \begin{array}{c} w \\ y \end{array} \right) \right), \quad D = \left( \begin{array}{ccc} \lambda^2 & -c^2 & 0 \\ 0 & 1 \end{array} \right) \]

\[ \text{ Inserting in (9) reads: } \]

\[ \partial_tE(t) + \int_{\Omega} \left( D \left( \begin{array}{cc} c & 0 \\ 0 & -c \end{array} \right) \partial_x \left( \begin{array}{c} w \\ y \end{array} \right), \left( \begin{array}{c} w \\ y \end{array} \right) \right) + \int_{\Omega} \left( DA \partial_{xxx} \left( \begin{array}{c} w \\ y \end{array} \right), \left( \begin{array}{c} w \\ y \end{array} \right) \right) = 0 \]

\[ \text{ integration by part gives: } \]

\[ \partial_tE(t) = 0. \]

\[ E(t) > 0 \text{ if } \lambda > c \Rightarrow \text{ subcharacteristic condition!} \]
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CLASSIC BOUNDARY CONDITIONS IN LBM CODES

The bounce-back condition

- **principle:** an incoming kinetic quantity gets the value of the outgoing kinetic quantity with opposite velocity. [Ziegler, 1993]
- **ex:** D2Q9 scheme:

  ![Diagram of bounce-back condition](image)

  \[
  f_1 = f_2, \quad f_3 = f_4, \\
  f_5 = f_6, \quad f_8 = f_7.
  \]

- Navier-Stokes equations: **no-slip** boundary conditions. [Cornubert et al., 1991]

Reflective conditions

- **principle:** the normal velocity only is null [Succi, 2001, Suswaram et al., 2015]
- **ex:** 3D2Q4 scheme for Euler, \( u \) is the normal velocity, and

  \[
  \rho = \sum f_i, \quad \rho u = \sum g_i, \quad \rho v = \sum h_i,
  \]

  then

  \[
  \rho u = \lambda (f_0 - f_1) = 0, \\
  \rho uv = \lambda (g_2 - g_3) = 0, \\
  \rho uv = \lambda (h_0 - h_1) = 0,
  \]

  provide the relations for the incoming kinetic quantities.

Other approaches

- the bounce-back and reflective conditions are not compatible with an implicit method,
- use of relaxation term towards a Dirichlet condition, [Coulette et al., 2018]
- **ex:** D1Q2 scheme and no-slip condition:

  \[
  \partial_t f_0 + \lambda \partial_x f_0 = \varepsilon^{-1} (f_0^{eq} - f_0) + \tau^{-1} (f_1 - f_0) \\
  \partial_t f_1 - \lambda \partial_x f_1 = \varepsilon^{-1} (f_1^{eq} - f_1) + \tau^{-1} (f_0 - f_1)
  \]
INFLOW/OUTFLOW CONDITIONS FOR THE OVER-RELAXATION SCHEME

Case of the 1D transport equation, but applies to all incoming waves.

Inflow condition

According to the equivalent equation, \( w \) is incoming, \( y \) is outgoing.

- imposed condition on \( w \):

\[
\frac{w_0^n + w_0^{n+1/4}}{2} = \nu(-c(t_n + \frac{\Delta t}{8})),
\]
INFLOW/OUTFLOW CONDITIONS FOR THE OVER-RELAXATION SCHEME

Case of the 1D transport equation, but applies to all incoming waves.

Outflow condition (at right boundary)

According to the equivalent equation, \( w \) is outgoing, \( y \) is incoming. Three strategies:

- **Exact strategy**: imposed condition on \( w \),
  \[
  \frac{w_{N+1}^n + w_{N+1}^{n+1/4}}{2} = v\left(1 - c(t_n + \frac{\Delta t}{8})\right).
  \]

- **Dirichlet strategy**: equilibrium value for \( z \),
  \[
  \frac{z_{N+1}^n + z_{N+1}^{n+1/4}}{2} - c\frac{w_{N+1}^n + w_{N+1}^{n+1/4}}{2} = 0,
  \]
  \[
  z_{N+1}^{n+1/4} - cw_{N+1}^{n+1/4} = z_N^{n+1/4} - cw_N^{n+1/4}.
  \]

- **Neumann strategy**: uniform disequilibrium \( \partial_x y = 0 \),
**NUMERICAL RESULTS - TRANSPORT EQUATION**

**Equation to be solved**

\[ \partial_t u + c \partial_x u = 0. \]

Initial condition:

\[ u(x, t) = \exp\left( A(x - \alpha - ct)^2 \right), \quad y(x, t) = 0, \]

with

\[ c = 1, \quad \lambda = 2, \quad t_{\text{max}} = 1, \quad \alpha = 0, \quad \beta = 0, \quad A = -80, \quad \text{and} \quad B = 0. \]

**Illustration**

**Convergence**
NUMERICAL RESULTS - EULER EQUATIONS

Equations to be solved (barotropic Euler)

\[
\frac{\partial t}{\partial t} u + \frac{\partial x}{\partial x} f(u) = 0
\]

\[
u = \begin{pmatrix} \rho \\ \rho v \end{pmatrix}, \quad f(u) = \begin{pmatrix} \rho v \\ \frac{(\rho v)^2}{\rho} + c^2 \rho \end{pmatrix}, \quad \rho > 0, \quad c = 10.
\]

Initial condition:

\[
\rho(x, 0) = \rho_0 + C \exp(D(x - x_0)), \quad (\rho v)(x, 0) = \rho(x, 0)v_0, \quad \rho_0 = 1.0, \quad v_0 = 3c.
\]

with

\[
C = 0.2, \quad D = -80, \quad x_0 = -0.5,
\]

and

\[
w_\rho(x, 0) = \rho(x, 0), \quad w_{\rho v}(x, 0) = (\rho v)(x, 0), \quad y_\rho(x, 0), y_{\rho v}(x, 0) = 0,
\]

Illustration

Convergence
CONCLUSION

Objectives:

▶ solve nonlinear systems of equations with HPC algorithms,
▶ ensure high-order and stable numerical schemes,
▶ deal with boundary conditions issues,
▶ simulate MHD physical problems.

Achievements:

▶ LBM and vectorial kinetic schemes show good compatibility with HPC (kirsch and patapon codes),
▶ time-symmetric and high-order in time schemes have been developed (the basic component being the over-relaxation scheme),
▶ the analysis of the equivalent equation of the over-relaxation scheme shows how to design compatible boundary conditions,
▶ 1D second-order boundary conditions have been developed.

Perspectives:

▶ 2D and 3D boundary conditions,
▶ analysis and boundary conditions for other kinetic schemes (ex: D1Q3) and LBM approaches.

Thank you for your attention!
CONCLUSION

Discrete kinetic schemes for multidimensional systems of conservation laws.

A fast and stable well-balanced scheme with hydrostatic reconstruction for shallow water flows.

A reduced stability condition for nonlinear relaxation to conservation laws.

Hyperbolic conservation laws with stiff relaxation terms and entropy.

A knudsen layer theory for lattice gases.

High-order implicit palindromic discontinuous galerkin method for kinetic-relaxation approximation.
submitted to JSC.

An analysis of over-relaxation in kinetic approximation.
submitted to Comptes Rendus Mécanique.


The relaxation schemes for systems of conservation laws in arbitrary space dimensions.

Composition constants for raising the orders of unconventional schemes for ordinary differential equations.

Splitting methods.
A discrete kinetic approximation of entropy solutions to multidimensional scalar conservation laws.

Boltzmann type schemes for gas dynamics and the entropy property.

The Lattice Boltzmann Equation for Fluid Dynamics and Beyond.

A lattice boltzmann relaxation scheme for inviscid compressible flows.
preprint.

Fractal decomposition of exponential operators with applications to many-body theories and monte carlo simulations.

Boundary conditions for lattice boltzmann simulations.