MHD simulations

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Part I: Conservation, Consistency, and Convergency
1 Linear and non-linear advection equations

We start with the continuity equation as the reference equation for advection:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 , \]

in 1-D

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

With \( u = \text{const.} \) (the advection velocity) we get the linear advection equation

\[ \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} = 0 . \]

Its solution is

\[ \rho(x, t) = \rho_0(x - ut) . \]
Linear and non-linear advection equations (cont.)

The initial density profile is simply moved (advected) with velocity $u$.

$\rho(x,t)$

$\rho_0(x)$

$\rho$ is a “generalized density”.

It is remarkable that Eulerian numerical schemes have generally difficulties to solve the linear advection equation accurately. Some amount of diffusion is unavoidable.

From Oran & Boris (1987)
Linear and non-linear advection equations (cont.)

We next consider the momentum equation

\[
\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2 + p) - \varepsilon \rho \frac{\partial^2 u}{\partial x^2} = 0 ,
\]

and assume \( p = 0 \):

\[
u \frac{\partial \rho}{\partial t} + \rho \frac{\partial u}{\partial t} + u^2 \frac{\partial \rho}{\partial x} + \rho 2u \frac{\partial u}{\partial x} - \varepsilon \rho \frac{\partial^2 u}{\partial x^2} = 0 .
\]

Using the continuity equation, the first term can be written as:

\[
u \frac{\partial \rho}{\partial t} = -u \frac{\partial}{\partial x} (u\rho) = -u^2 \frac{\partial \rho}{\partial x} - \rho \frac{\partial u}{\partial x}
\]

\[
\Rightarrow \rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} - \rho \varepsilon \frac{\partial^2 u}{\partial x^2} = 0 .
\]

Division by \( \rho \) and reordering terms leads to:
Linear and non-linear advection equations (cont.)

Burgers’ equation

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \varepsilon \frac{\partial^2 u}{\partial x^2}
\]

and the inviscid Burgers’ equation

\[
u_t + uu_x = 0
\]
Linear and non-linear advection equations (cont.)

Burgers’ equation

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \epsilon \frac{\partial^2 u}{\partial x^2} \]

and the inviscid Burgers’ equation

\[ u_t + uu_x = 0 \]
Linear and non-linear advection equations (cont.)

Solutions to the inviscid Burgers equation $u_t + uu_x = 0$:

\[ u(x,t) \]

$u(x,0)$

Solutions to the Burgers equation $u_t + uu_x = \varepsilon u_{xx}$:

$\varepsilon = 0.01$

$\varepsilon = 0.005$

$\varepsilon \to 0$

limiting solution as $\varepsilon \to 0$

$\varepsilon = 0.005$

$\varepsilon = 0.01$
Consider the inviscid Burgers equation \( u_t + uu_x = 0 \) with the initial data

\[
    u_0 = \begin{cases} 
    1 & \text{for } x \leq 0 \\
    0 & \text{for } x > 0
    \end{cases}
\]

and construct a straightforward discretization:

\[
    \frac{U_j^{n+1} - U_j^n}{k} + U_j^n \left( \frac{U_j^n - U_{j-1}^n}{h} \right) = 0 ,
\]

which is an ‘upwind” or “donor cell” scheme. How does this scheme handle the discontinuity of the initial data?
Linear and non-linear advection equations (cont.)

First we rewrite the scheme in explicite form:

\[ U_{j}^{n+1} = U_{j}^{n} - \frac{k}{h} U_{j}^{n} (U_{j}^{n} - U_{j-1}^{n}) . \]

Next we compute the first time step:

- for \( x < 0 \) : \( U_{j}^{1} = 1 - \frac{k}{h} 1 (1 - 1) = 1 \),
- for \( x > 0 \) : \( U_{j}^{1} = 0 - \frac{k}{h} 0 (0 - 0) = 0 \),
- for \( U_{j-1} = 1 \) and \( U_{j} = 0 \) : \( U_{j}^{1} = 0 - \frac{k}{h} 0 (0 - 1) = 0 \).
Linear and non-linear advection equations (cont.)

First we rewrite the scheme in explicit form:

\[ U_{j}^{n+1} = U_{j}^{n} - \frac{k}{h} U_{j}^{n} (U_{j}^{n} - U_{j-1}^{n}) . \]

Next we compute the first time step:

for \( x < 0 \) : \( U_{1}^{1} = 1 - \frac{k}{h} 1 (1 - 1) = 1 , \)

for \( x > 0 \) : \( U_{1}^{1} = 0 - \frac{k}{h} 0 (0 - 0) = 0 , \)

for \( U_{j-1} = 1 \) and \( U_{j} = 0 \) : \( U_{j}^{1} = 0 - \frac{k}{h} 0 (0 - 1) = 0 . \)

⇒ After one time step we recover the initial data again!

Whatever step size \( h \) and \( k \) we choose, the shock front stays at the same position.
True (solid curve) and computed (dotted curve) solution to Burgers’ equation with adjacent initial data and using the upwind scheme. Note that the shock speed is wrong.

\[ u_0 = \begin{cases} 
1.2 & \text{for } x \leq 0 \\
0.4 & \text{for } x > 0 
\end{cases} \]
Def.: A scheme is in *conservation law form* if it has the form

\[ U_j^{n+1} = U_j^n - \frac{k}{h} \left[ F(U_{j-p}^n, U_{j-p+1}^n, \cdots, U_{j+q}^n) ight. \]

\[ \left. - F(U_{j-p-1}^n, U_{j-p}^n, \cdots, U_{j+q-1}^n) \right] . \]

*F* is called the *numerical flux function*. 

\[ \]
Conservative methods (cont.)

A good way to obtain conservation law form is to start discretization from the conservative form of the PDE.

For example in case of the inviscid Burgers equation:

\[
\text{quasi linear form} \quad : \quad u_t + uu_x = 0 ,
\]

\[
\text{conservative form} \quad : \quad u_t + \left(\frac{1}{2}u^2\right)_x = 0 .
\]

Using the same upwind discretization as before but starting from the conservative form of the PDE we obtain:

\[
\frac{U_j^{n+1} - U_j^n}{k} + \frac{1}{h} \left[ \frac{1}{2}(U_j^n)^2 - \frac{1}{2}(U_{j-1}^n)^2 \right] = 0 .
\]
The explicit form is

\[ U_{j}^{n+1} = U_{j}^{n} - \frac{k}{h} \left[\frac{1}{2}(U_{j}^{n})^2 - \frac{1}{2}(U_{j-1}^{n})^2\right] = 0 , \]

which is distinctly different from the difference equation that we had before:

\[ U_{j}^{n+1} = U_{j}^{n} - \frac{k}{h} U_{j}^{n} (U_{j}^{n} - U_{j-1}^{n}) . \]

The first equation has the form

\[ U_{j}^{n+1} = U_{j}^{n} - \frac{k}{h} \left[ F(U_{j}^{n}) - F(U_{j-1}^{n}) \right] , \]

hence, it is in conservation law form according to the definition. Applying it to the same initial data as before produces the correct solution with the correct shock speed.
Conservative methods (cont.)

True (solid curve) and computed (dotted curve) solution to Burgers’ equation with adjacent initial data and using the conservative upwind scheme. Note that the shock speed is correct.

\[ u_0 = \begin{cases} 
1.2 & \text{for } x \leq 0 \\
0.4 & \text{for } x > 0 
\end{cases} \]
§ 3 Conservation, Consistency, Convergence

Def.: $U^n_j$: numerical solution at grid point $j$ and time $t = (n - 1)k$ ($k = \Delta t$)

$u^n_j: = u(x_j, t_n)$ exact solution at grid point $j$ and time $t = (n - 1)k$

$\mathcal{H}_k$: explicit numerical scheme using time steps $k$ so that

$$U^{n+1} = \mathcal{H}_k(U^n)$$

$L_k$: local truncation error

$$L_k(x_j, t) = \frac{1}{k} [u(x_j, t + k) - \mathcal{H}_k(u(\cdot, t); x_j)]$$

Then, a method is consistent if $\|L_k(\cdot, t)\| \to 0$ as $k \to 0,$

where $\|v\| := \int_{-\infty}^{\infty} |v(x)| \, dx$, while $k/h = \text{const}$
A scheme in conservation law form

\[ U_{j}^{n+1} = U_{j}^{n} - \frac{k}{h} \left[ F(U_{j-p}^{n}, U_{j-p+1}^{n}, \ldots, U_{j+q}^{n}) \right. \]
\[ \left. - F(U_{j-p-1}^{n}, U_{j-p}^{n}, \ldots, U_{j+q-1}^{n}) \right] \]

is consistent with the conservative PDE

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

if

\[ F(u, u, \ldots, u) = f(u) \]

and there exists a \( K \) such that

\[ |F(U_{j-p}, \ldots, U_{j+q}) - f(u)| \leq K \max_{-p \leq i \leq q} |U_{j+1} - u|. \]
For example Burgers’ equation and its conservative upwind scheme are consistent:

\[ F(U_j) = \frac{1}{2} (U_j)^2 \Rightarrow F(u) = \frac{1}{2} u^2 = f \]

This scheme is conservative \textit{and} consistent!
Theorem of Lax and Wendroff (1960)

Consider a sequence of grids, indexed by \( l = 1, 2, \ldots \) with mesh parameters \( k_l, h_l \to 0 \) as \( l \to \infty \). Let \( U_l(x, t) \) denote the numerical solution computed with a consistent and conservative method on the \( l \)th grid. Suppose that \( U_l \) converges* to a function \( u \) as \( l \to \infty \). Then \( u(x, t) \) is a weak solution of the conservation law.

* Convergence in the following sense:

Over every bounded set \( \Omega = [a, b] \times [0, T] \)

\[
\int_0^T \int_a^b |U_l(x, t) - u(x, t)| \, dx \, dt \to 0 \text{ as } l \to \infty
\]

and

\[
\text{TV}(U(\cdot, t)) < R \quad 0 \leq t \leq T, \quad l = 1, 2, \ldots
\]

where

\[
\text{TV}(v) = \sup \sum_{j=1}^N \left| v(\xi_j) - v(\xi_{j-1}) \right|
\]
§ 4 Theorem of Godunov

Def.: If we have initial data that are monotone increasing or decreasing, e.g.,

\[ U_j^0 \geq U_{j+1}^0 \quad \forall j \quad \text{(monotonically decreasing)} \]

and the numerical scheme produces solutions with

\[ U_j^n \geq U_{j+1}^n \quad \forall j \quad \text{and} \quad n, \]

then the scheme is said to be \textit{monotone}.

For example, the upwind scheme is a monotone scheme.

\textbf{Theorem of Godunov (1959)}

A \textit{linear, monotonicity preserving} method is at most \textit{first order} accurate.

A scheme \( \mathcal{H} \) is linear if

\[ \mathcal{H}(U + V) = \mathcal{H}(U) + \mathcal{H}(V). \]

(It has the general form

\[ U_i^{n+1} = \sum_{k=-k_L}^{k_R} b_k U_{i+k}^n, \quad k_L, k_R \in \mathbb{N}^+ \] )
References


Part II: Riemann solvers
Three major progresses in computational fluid dynamics of the past 50 years include:

- the \textit{conservative formulation} of the computational scheme in terms of finite volumes,
- the technique of approximate \textit{Riemann-solvers} for the computation of numerical fluxes,
- the \textit{flux-limiter} technique for maintaining stability and monotonicity of higher-order accurate scheme.
Consider the continuity equation:

$$
\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0 .
$$

(1)

Integration over a finite volume, $\mathcal{V}$, and time period, $T$, leads to the integral form of this equation:

$$
\int_{\mathcal{V}} \rho(T, \mathbf{x}) dV - \int_{\mathcal{V}} \rho(0, \mathbf{x}) dV = \int_0^T \oint_{\partial \mathcal{V}} (\rho \mathbf{u}) \cdot \mathbf{n} ds dt
$$

(2)

Solutions to Eq. (2) are called weak solutions to the partial differential equation, Eq. (1). Additionally to the solutions of Eq. (1), the set of solutions to Eq. (2) encompasses discontinuous solutions, because no derivatives appear in Eq. (2). Discontinuous solutions to the Euler equations represent shock fronts of the real world.
Conservation laws – finite volumes (cont.)

Consider the mass conservation in a one-dimensional tube:

\[
m(t + \Delta t) = m(t) + \langle \rho v \rangle_1 A \Delta t - \langle \rho v \rangle_2 A \Delta t
\]

Eq. (3) is identical to the integral form Eq. (2):

\[
\int_V \rho(T, x) dV - \int_V \rho(0, x) dV = \int_0^T \oint_{\partial V} (\rho \mathbf{u}) \cdot \mathbf{n} \, ds \, dt
\]

Eq. (4) has the form of a \textit{conservative finite volume scheme}. In the limit of \( \Delta x \to 0 \) and \( \Delta t \to 0 \):

\[
\frac{\partial \rho}{\partial t} = \frac{\partial (\rho u)}{\partial x}
\]
Conservation laws – finite volumes (cont.)

The conservative, finite volume formulation has three highly desirable properties:

– Conserved quantities (mass, momentum, energy) remain accurately conserved

– Discontinuous solutions are include by solving the integral form of the partial differential equation

– It fulfills one of two requirements of the theorem of Lax and Wendroff (1960) that says:

The approximate solution that is computed with a *consistent* and *conservative* scheme *converges* to a weak solution of the conservation law.
Euler’s equation in one dimension is given by

\[ q_t + f(q)_x = 0 , \quad q^{n+1}_i = q^n_i + \frac{\Delta t}{\Delta x} [f_{i-1/2} - f_{i+1/2}] , \]

where

\[
q = \begin{pmatrix}
\rho \\
\rho u \\
E
\end{pmatrix} \quad f(q) = \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
u(E + p)
\end{pmatrix}
\]

In 3-D we have

\[ q_t + f(q)_x + g(q)_y + h(q)_z = 0 , \]

with

\[
q = \begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
E
\end{pmatrix} \quad f(q) = \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho uw \\
u(E + p)
\end{pmatrix} \quad \ldots
\]
A conservative finite volume scheme is an exact representation of the integral form of the partial differential equation of the conservation law. The problem consists in computing the correct flux function $f(q)$, i.e., $\langle \rho v \rangle$ in the case of the continuity equation.

It turns out that these fluxes can be computed exactly.
Riemann solvers (cont.)

Idea of S.K. Godunov (1959): Piecewise constant reconstruction with discontinuities at cell interfaces
Riemann solvers (cont.)

The shock-tube problem

\[ p_l \quad p_r \]
\[ \rho_l \quad \rho_r \]
\[ v_l = v_r = 0 \]
Riemann solvers (cont.)

The shock-tube problem

\[ p_l \quad \rho_l \quad v_l = 0 \quad t_0 \]

\[ p_r \quad \rho_r \quad v_r \]

\[ p_l \quad \rho_l \quad p_l^* \quad \rho_l^* \quad \rho_r \quad v_r^* \quad t_1 \]

\[ p_r \quad \rho_r \quad \rho_r^* \]

\[ v_l \quad v_r \]
Riemann solvers (cont.)

The shock-tube problem

\[ \rho_l \quad \rho_r \]
\[ \begin{align*}
    p_l \quad & p_r \\
    v_l \quad & v_r = 0
\end{align*} \]

\[ \rho_l \quad \rho_r \]
\[ \begin{align*}
    p_l \quad & p_r^* \\
    v_l \quad & v_r^*
\end{align*} \]

\[ \begin{align*}
    \rho_l \quad & \rho_r \quad \rho_r^* \\
    p_l \quad & p_r \quad v_r
\end{align*} \]
The shock-tube problem

\[ p_l \quad \rho_l \quad v_l = v_r = 0 \quad q_0 = q_r \]

\[ p_r \quad \rho_r \quad v_r \quad q_r \]

\[ p_l^* \quad \rho_l^* \quad v_l^* \quad q_l^* \]

\[ p_r^* \quad \rho_r^* \quad v_r^* \quad q_r^* \]

\[ \Delta t \]

\[ q_0 = q_r \quad q_0 = q_r^* \quad q_0 = q_l^* \quad q_0 = q_{rf} \quad q_0 = q_l \]
Consider the system of one-dimensional conservation laws

\[ q_t + f(q)_x = 0, \quad q(x, 0) = \begin{cases} q_l & \text{if } x < 0, \\ q_r & \text{if } x > 0. \end{cases} \]

The integral form in the control volume \([x_l, x_r] \times [0, T]\) is given by:

\[
\int_{x_l}^{x_r} q(x, T) \, dx = \int_{x_l}^{x_r} q(x, 0) \, dx + \int_0^T f(q(x_l, t)) \, dt - \int_0^T f(q(x_r, t)) \, dt
\]
The HLL solver (cont.)

\[
\int_{x_l}^{x_r} q(x, T) \, dx = \int_{x_l}^{x_r} q(x, 0) \, dx + \int_0^T f(q(x_l, t)) \, dt - \int_0^T f(q(x_r, t)) \, dt \\
= x_r q_r - x_l q_l + T(f_l - f_r), \quad f_l = f(q_l), \quad f_r = f(q_r)
\]

\[
\int_{x_l}^{x_r} q(x, T) \, dx = \int_{x_l}^{T_{s_l}} q(x, T) \, dx + \int_{T_{s_l}}^{T_{s_r}} q(x, T) \, dx + \int_{T_{s_r}}^{x_r} q(x, T) \, dx \\
= \int_{T_{s_l}}^{T_{s_r}} q(x, T) \, dx + (T_{s_l} - x_l)q_l + (x_r - T_{s_r})q_r
\]

\[
\frac{1}{T(s_r - s_l)} \int_{T_{s_l}}^{T_{s_r}} q(x, T) \, dx \ := \ \mathbf{q}^{hll} = \frac{s_r q_r - s_l q_l + f_l - f_r}{s_r - s_l}
\]
The HLL solver (cont.)

Applying the integral form to the control volume $[x_l, 0] \times [0, T]$ we obtain:

$$\int_{T s_l}^{0} q(x, T) \, dx = -T s_l q_l + T (f_l - f_{0l}) ,$$

where $f_{0l}$ is the flux $f(q)$ along the $t$-axis. Hence,

$$f_{0l} = f_l - s_l q_l - \frac{1}{T} \int_{T s_l}^{0} q(x, T) \, dx .$$

Doing the same for the control volume $[0, x_r] \times [0, T]$ leads to

$$f_{0r} = f_r - s_r q_r - \frac{1}{T} \int_{0}^{T s_r} q(x, T) \, dx .$$

It follows that

$$f_{0l} = f_{0r} .$$
Harten, Lax, and van Leer put forward the following approximation:

\[ \tilde{q}(x, t) = \begin{cases} 
q_l & \text{if } \frac{x}{t} \leq s_l , \\
q_{\text{hll}} & \text{if } s_l \leq \frac{x}{t} \leq s_r , \\
q_r & \text{if } \frac{x}{t} \geq s_r . 
\end{cases} \]

\[ f_{\text{hll}} = f_l + s_l(q_{\text{hll}} - q_l) \quad \text{or} \]
\[ f_{\text{hll}} = f_r + s_r(q_{\text{hll}} - q_r) \]

\[ \Rightarrow f_{\text{hll}} = \frac{s_r f_l - s_l f_r + s_l s_r (q_r - q_l)}{s_r - s_l} \]
The HLL solver (cont.)

The corresponding intercell flux for the approximate Godunov method is then given by:

\[
\begin{align*}
  f_{i+1/2}^{hll} &= \begin{cases} 
    f_l, & \text{if } 0 \leq s_l, \\
    s_r f_l - s_l f_r + s_l s_r (q_r - q_l), & \text{if } s_l \leq 0 \leq s_r, \\
    f_r, & \text{if } 0 \geq s_r,
  \end{cases}
\end{align*}
\]

that can be used in the explicit conservative formula

\[
q_i^{n+1} = q_i^n + \frac{\Delta t}{\Delta x} \left[ f_{i-1/2} - f_{i+1/2} \right].
\]
7.2 Wave-speed estimates

In order to completely determine the numerical fluxes in the HLL Riemann solver we need estimates for the wave speeds $s_l$ and $s_r$, and, for the HLLC solver, $s^*$. Given a positive speed $s^+$, a simple choice would consist in

$$s_l = -s^+, \quad s_r = s^+.$$

It is interesting to note that if we set $s^+$ equal to the maximal speed according to the CFL-condition, i.e.,

$$s^+ = \frac{\Delta x}{\Delta t},$$

we obtain Lax-Friederichs numerical flux

$$f_{i+1/2} = \frac{1}{2}(f_l - f_r) - \frac{1}{2} \frac{\Delta x}{\Delta t}(q_r - q_l),$$

which brings us back to a classical scheme.
Wave-speed estimates (cont.)

More ingenious choices are motivated by a “Roe average” of the left and right states, e.g.,

\[ s_l = \tilde{u} - \tilde{a}, \quad s_r = \tilde{u} + \tilde{a}, \]

where

\[ \tilde{u} = \frac{\sqrt{\rho_l u_l} + \sqrt{\rho_r u_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}}, \quad \tilde{a} = \left[ (\gamma - 1)(\tilde{H} - \frac{1}{2}\tilde{u}^2) \right]^{\frac{1}{2}}, \]

with the enthalpy \( H = (E + p)/\rho \) approximated as

\[ \tilde{H} = \frac{\sqrt{\rho_l H_l} + \sqrt{\rho_r H_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}}. \]
Wave-speed estimates (cont.)

In a different approach we first suppose to have estimates for $p^*$ and $u^*$ for the pressure and velocity in the Star Region. Then we compute the following wave speeds:

$$s_l = u_l - a_l r_l , \quad s^* = u^* , \quad s_r = u_r + a_r r_r ,$$

where

$$r_k = \begin{cases} 
1 & \text{if } p^* \leq p_k \quad \text{rarefaction head} \\
\left[ 1 + \frac{\gamma + 1}{2\gamma} \left( \frac{p^*}{p_k} - 1 \right) \right]^{\frac{1}{2}} & \text{if } p^* > p_k \quad \text{shock}
\end{cases}$$

$p^*$ and $u^*$ can be found from a linearization of the Riemann problem yielding

$$p^* = \frac{1}{2} (p_l + p_r) - \frac{1}{2} (u_r - u_l) \bar{\rho} \bar{a} , \quad u^* = \frac{1}{2} (u_l + u_r) - \frac{1}{2} \left( \frac{p_r - p_l}{\bar{\rho} \bar{a}} \right) ,$$

where

$$\bar{\rho} = \frac{1}{2} (\rho_l + \rho_r) , \quad \bar{a} = \frac{1}{2} (a_l + a_r) .$$
Consider again the Riemann problem

\[ q_t + f(q)_x = 0, \]

\[ q(x, 0) = \begin{cases} 
q_l & \text{if } x < 0, \\
q_r & \text{if } x > 0,
\end{cases} \]

where for the \( x \)-split three-dimensional Euler equation

\[ q = \begin{pmatrix} 
\rho \\
\rho u \\
\rho v \\
\rho w \\
E
\end{pmatrix}, \quad f(q) = \begin{pmatrix} 
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho uw \\
u(E + p)
\end{pmatrix}. \]
The Roe solver (cont.)

Using the chain rule, the conservation law

\[ q_t + f(q)_x = 0 \]

may be written as

\[ q_t + A(q)q_x = 0, \quad A(q) = \frac{\partial f}{\partial q}. \]

Roe’s approach consists in replacing the Jacobian matrix \( A(q) \) by a constant Jacobian

\[ \tilde{A} = \tilde{A}(q_l, q_r) \]

resulting in the Riemann problem for the linear system

\[ q_t + \tilde{A}q_x = 0, \]

\[ q(x, 0) = \begin{cases} q_l & \text{if } x < 0, \\ q_r & \text{if } x > 0, \end{cases} \]

which can be solved exactly.
The Roe solver (cont.)

Once the matrix $\tilde{A}(q_l, q_r)$, its eigenvalues $\tilde{\lambda}_i(q_l, q_r)$, and corresponding right eigenvectors $\tilde{k}^{(i)}(q_l, q_r)$ are available, the difference between right and left state can be expanded in terms of the eigenvectors:

$$\Delta q = q_r - q_l = \sum_{i=1}^{m} \tilde{\alpha}_i \tilde{k}^{(i)},$$

from which one finds the wave strengths $\tilde{\alpha}_i(q_l, q_r)$.

$$q_{i+1/2}(0) = q_l + \sum_{\tilde{\lambda}_i \leq 0} \tilde{\alpha}_i \tilde{k}^{(i)}, \quad \text{or}$$

$$q_{i+1/2}(0) = q_r - \sum_{\tilde{\lambda}_i \geq 0} \tilde{\alpha}_i \tilde{k}^{(i)},$$

$$f_{i+1/2} = f_l + \sum_{\tilde{\lambda}_i \leq 0} \tilde{\alpha}_i \tilde{\lambda}_i \tilde{k}^{(i)}, \quad \text{or}$$

$$f_{i+1/2} = f_r - \sum_{\tilde{\lambda}_i \geq 0} \tilde{\alpha}_i \tilde{\lambda}_i \tilde{k}^{(i)}.$$
The Roe solver (cont.)

The $x$-direction Jacobian matrix for the Euler equations, $A(q)$, is

$$A = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
\hat{\gamma}H - u^2 - a^2 & (3 - \gamma)u & -\hat{\gamma}v & -\hat{\gamma}w & \hat{\gamma} \\
-uv & v & u & 0 & 0 \\
-wv & w & 0 & u & 0 \\
\frac{1}{2}u[(\gamma - 3)H - a^2] & H - \hat{\gamma}u^2 & -\hat{\gamma}uv & -\hat{\gamma}uw & \gamma u
\end{bmatrix},$$

where $\hat{\gamma} = \gamma - 1$ and $a = \sqrt{\gamma p/\rho}$. The eigenvalues are

$$\lambda_1 = u - a, \quad \lambda_2 = \lambda_3 = \lambda_4 = u, \quad \lambda_5 = u + a.$$
The Roe solver (cont.)

The corresponding right eigenvalues are

\[
\begin{align*}
k^{(1)} &= \begin{bmatrix} 1 \\ u - a \\ v \\ w \\ H - ua \end{bmatrix}, &
k^{(2)} &= \begin{bmatrix} 1 \\ u \\ v \\ w \\ \frac{1}{2} V^2 \end{bmatrix}, &
k^{(3)} &= \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ v \end{bmatrix}, \\
k^{(4)} &= \begin{bmatrix} 0 \\ 0 \\ 1 \\ w \end{bmatrix}, &
k^{(5)} &= \begin{bmatrix} 1 \\ u + a \\ v \\ w \\ H + ua \end{bmatrix},
\end{align*}
\]

where

\[
H = \frac{E + p}{\rho}, \quad E = \frac{1}{2}\rho V^2 + \rho e, \quad V^2 = u^2 + v^2 + w^2.
\]
The Roe solver (cont.)

Roe requires the constant Jacobian matrix $\tilde{A} = \tilde{A}(q_l, q_r)$ to satisfy the algebraic properties of the Jacobian $A(q)$, i.e.,

$$\tilde{\lambda}_i = \tilde{\lambda}_i(q_l, q_r) \in \mathbb{R} \quad \forall i,$$

$$\tilde{A}(q, q) = A(q),$$

$$f(q_r) - f(q_l) = \tilde{A}(q_r - q_l).$$

These conditions may be fulfilled with the following “Roe averaged” quantities to be used in the formulae for $\lambda_i$ and $k^{(i)}$ shown on the previous pages:

$$\tilde{u} = \frac{\sqrt{\rho_l u_l} + \sqrt{\rho_r u_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}},$$

$$\tilde{H} = \frac{\sqrt{\rho_l H_l} + \sqrt{\rho_r H_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}},$$

$$\tilde{v} = \frac{\sqrt{\rho_l v_l} + \sqrt{\rho_r v_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}},$$

$$\tilde{\alpha} = (\gamma - 1)[\tilde{H} - \frac{1}{2}\tilde{V}^2]\frac{1}{\tilde{\rho}},$$

$$\tilde{w} = \frac{\sqrt{\rho_l w_l} + \sqrt{\rho_r w_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}},$$

$$\tilde{V}^2 = \tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2.$$
§ 8 Higher order accurate methods

Piece-wise linear, local reconstruction (variable extrapolation method) as part of the MUSCL scheme (Monotone Upstream-centred Scheme for Conservation Laws)

\[ q_i(x) = q_i^n + \frac{x - x_i}{\Delta x} \Delta_i \quad x \in [0, \Delta x], \]

\[ q_i^L = q_i^n - \frac{1}{2} \Delta_i, \]

\[ q_i^R = q_i^n + \frac{1}{2} \Delta_i, \]

leads to the Generalized Riemann Problem

\[ q_t + f(q)_x = 0, \]

\[ q(x, 0) = \begin{cases} 
q_i(x) & \text{if } x < 0, \\
q_{i+1}(x) & \text{if } x > 0.
\end{cases} \]
TVD methods (cont.)

Initial data (a) and solution structure (b) of the generalized Riemann problem.

In the MUSCL-Hancock method intermediate boundary extrapolated values $\tilde{q}_{i}^{R}$ and $\tilde{q}_{i+1}^{L}$ are obtained by

$$\tilde{q}_{i}^{L} = q_{i}^{L} + \frac{1}{2} \frac{\Delta t}{\Delta x} [f(q_{i}^{L}) - f(q_{i}^{R})],$$
$$\tilde{q}_{i}^{R} = q_{i}^{R} + \frac{1}{2} \frac{\Delta t}{\Delta x} [f(q_{i}^{L}) - f(q_{i}^{R})],$$

which then form the piece-wise constant data for the conventional Riemann problem

$$q_{t} + f(q)_{x} = 0,$$
$$q(x, 0) = \begin{cases} 
\tilde{q}_{i}^{R} & \text{if } x < 0, \\
\tilde{q}_{i+1}^{L} & \text{if } x > 0.
\end{cases}$$
TVD methods (cont.)

An important property of the general scalar conservation law

\[ u_t + f(u)_x = 0 \]  \hspace{1cm} (5)

is monotoncity:

If two initial data functions \( v_0(x) \) and \( u_0(x) \) for Eq. (5) satisfy \( v_0(x) \geq u_0(x) \) \( \forall x \),
then the corresponding solutions \( v(x, t) \) and \( u(x, t) \) satisfy \( v(x, t) \geq u(x, t) \) \( t > 0 \).

Correspondingly, a monotone scheme has the following property:

\[ \text{if } \quad v_i^n \geq u_i^n \quad \forall i \quad \text{then} \quad v_i^{n+1} \geq u_i^{n+1} \quad \forall i. \]

The Theorem of Godunov states that: There are no monotone, linear schemes for the solution of Eq. (5) of second or higher order of accuracy.

(A linear scheme has generally the form

\[ q_i^{n+1} = \sum_{k=-k_L}^{k_R} b_k q_{i+k}^n, \quad k_L, k_R \in \mathbb{N}^+ \)
TVD methods (cont.)

In order to circumvent Godunov’s theorem, higher order *non-linear* schemes were invented. One way of doing so consists in finding a *slope limiter* $\xi_i$ such that

$$\bar{\Delta}_i = \xi_i \Delta_i,$$

$$\Delta_i = \frac{1}{2} (1 + \omega) (q^n_i - q^n_{i-1}) + \frac{1}{2} (1 + \omega) (q^n_{i+1} - q^n_i), \quad \omega \in [-1, 1].$$

$\xi_i$ depends in a non-linear way on the ratio $r$, where

$$r = \frac{q^n_i - q^n_{i-1}}{q^n_{i+1} - q^n_i}$$

TVD region for slope limiters. For negative $r$ the TVD region is the single line $\xi = 0$, for positive $r$ the TVD region corresponds to the pink region. SUPERBEE, van Leer, MINMOD, etc type of slope limiters are a subset of this region.
The positivity problem with HLL when applied to MHD

The HLL-scheme is a positive scheme when applied to the system of the Euler equations. This means that density and pressure remain positive under all circumstances.

It remains positive when applied to the system of one-dimensional MHD equations as long as the longitudinal magnetic field component is continuous, i.e., constant. The transversal components may have discontinuities.

The HLL-middle state can become non-positive if there is a jump in the normal component of the magnetic field across the cell interface.
The positivity problem with HLL when applied to MHD (cont.)

In planar MHD the solenoidality condition reduces to

$$\frac{\partial B_x}{\partial x} = 0,$$

since $B_y$ and $B_z$ are constant in the transversal directions $y$ and $z$. Hence, $B_x(x) = \text{const}$. However, in multiple dimensions, this need not be the case any more.
The positivity problem with HLL when applied to MHD (cont.)

However, many multidimensional codes work with *dimensional operator splitting*, where numerical updates are computed separately for each dimensional direction. Each “directional sweep” is treated as a purely one-dimensional problem.

The *problem* with directional splitting in multi-dimensional MHD is that the one-dimensional sweeps “see” at cell boundaries discontinuities in the longitudinal component of the magnetic field.
Remedy proposed by Janhunen (2000): Discontinuities in the normal component of the magnetic field in planar MHD lead to the violation of the solenoidality condition, hence, they signify *magnetic monopoles*. Since we cannot avoid these discontinuities we modify the MHD equations in a way that they include magnetic monopoles.
The MHD-equations can be derived without using the condition $\nabla \cdot \mathbf{B} = 0$ at first. Powell (1994) derived the following set of equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot \left[ \rho \mathbf{v} \mathbf{v} + (p + \frac{B^2}{2\mu_0})\mathbb{I} - \frac{1}{\mu_0} \mathbf{B} \mathbf{B} \right] = -\mathbf{B} (\nabla \cdot \mathbf{B})$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{v} \mathbf{B} - \mathbf{B} \mathbf{v}) = -\mathbf{v} (\nabla \cdot \mathbf{B})$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left[ (E + p + \frac{B^2}{2\mu_0})\mathbf{v} - \frac{1}{\mu_0} (\mathbf{v} \cdot \mathbf{B}) \mathbf{B} \right] = -(\mathbf{v} \cdot \mathbf{B}) (\nabla \cdot \mathbf{B})$$

Powell used this system in order to avoid the accumulation of numerical discretization errors in $\nabla \cdot \mathbf{B}$. 
Janhunen argues that Powell’s monopols were ghost particles with no interaction with the electromagnetic field. The “correct way” to derive monopole MHD would include a force on magnetic monopoles in a similar way as electric charges experience a force in a electric field. He uses a generalization of the Lorentz force and so obtains:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0
\]

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot \left[ \rho \mathbf{v} \mathbf{v} + \left( p + \frac{B^2}{2\mu_0} \right) \mathbb{I} - \frac{1}{\mu_0} \mathbf{B} \mathbf{B} \right] = 0
\]

\[
\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{v} \mathbf{B} - \mathbf{B} \mathbf{v}) = -\mathbf{v} (\nabla \cdot \mathbf{B})
\]

\[
\frac{\partial E}{\partial t} + \nabla \cdot \left[ (E + p + \frac{B^2}{2\mu_0}) \mathbf{v} - \frac{1}{\mu_0} (\mathbf{v} \cdot \mathbf{B}) \mathbf{B} \right] = 0
\]

The linearized system has an eigenstructure similar to Powell’s equations.
The positivity problem with HLL when applied to MHD (cont.)

Janhunen correspondingly includes a source term in the HLL-solver for the induction equation:

\[ s_{B}^{\text{hll}} = \int_{0}^{T} \frac{1}{L} \int_{s_{l}T}^{s_{r}T} s(x, t) \, dx \, dt \]

\[ \approx \int_{0}^{T} \frac{1}{L} \int_{s_{l}T}^{s_{r}T} (-v_{hll} \frac{\partial B_{x}}{\partial x}) \, dx \, dt \]

\[ = \int_{0}^{T} \frac{1}{L} \int_{s_{l}T}^{s_{r}T} (-v_{hll} \frac{\partial B_{x}}{\partial x}) \, dx \, dt \]

\[ = \frac{1}{s_{r} - s_{l}} \int_{0}^{T} (-v_{hll}) \Delta B_{x} \, dt \]

\[ = -\frac{v_{hll} \Delta B_{x}}{s_{r} - s_{l}} \]

where \( L = (s_{r} - s_{l})T \) and \( \Delta B_{x} = B_{x_{r}} - B_{x_{l}} \). The only approximation involved is \( v \approx v_{hll} \).
Notice, that the “Janhunen trick” is used only for computing cell centered magnetic field components, which in turn are only used for computing numerical fluxes. The magnetic field proper of the solution is defined at cell boundaries and updated with a constrained transport (CT) scheme, which strictly maintains $\nabla \cdot \mathbf{B}$. 
The positivity problem with HLL when applied to MHD (cont.)

Even when using the Janhunen source term we have encountered instances of *negative pressure* when $\beta_{\text{plasma}} \ll 1$. In these cases the total energy is completely dominated by the magnetic energy, so that the internal energy may become negative when computing it by subtraction of the magnetic from the total energy.

We therefore use a *hybrid scheme* in the MHD-module of the CO$^5$ BOLD code. In regions with $\beta_{\text{plasma}} \ll 1$ we use the equation for internal energy instead of the total energy equation. We thereby *violate strict energy conservation*. In all other regions the total energy equation is used. The switch from total to internal energy equation can be specified as a parameter. A typical value would be $\beta_{\text{switch}} = 10^{-3}$. 
References

Part III: Concrete implementations
In the following is a non-exhaustive, arbitrarily selected list of codes that may or may not be suitable for serving your needs. Details are without guarantee.

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<th>acronym</th>
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<th>radiative transfer</th>
<th>parallelization</th>
<th>grid</th>
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<td>VAC</td>
<td>Versatile Advection Code</td>
<td><a href="http://www.phys.uu.nl/~toth/">http://www.phys.uu.nl/~toth/</a></td>
<td>Gábor Tóth</td>
<td>dimension independent notation, (convertible to FORTRAN via VAC Preprocessor)</td>
<td>yes</td>
<td>no</td>
<td>HPF, MPI, OpenMP</td>
<td>structured grid; adaptive/AMR</td>
<td>The code features a variety of numerical methods for the advection step including TVD schemes and Riemann solvers. There is a version with automatic adaptive mesh refinement, AMR.</td>
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<td><a href="http://www.nordita.org/software/pencil-code/">http://www.nordita.org/software/pencil-code/</a></td>
<td>Wolfgang Dobler</td>
<td>FORTRAN</td>
<td>yes</td>
<td>yes</td>
<td>MPI</td>
<td>Cartesian; adaptive/static</td>
<td>Code uses a higher order finite-difference scheme. Primarily designed to deal with weakly compressible turbulent flows.</td>
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<td><strong>CO</strong>&lt;sup&gt;5&lt;/sup&gt; BOLD</td>
<td>Conservative Code for the Computation of Compressible Convection in a Box of L Dimensions</td>
<td><a href="http://www.astro.uu.se/~bf/co5bold_main.html">http://www.astro.uu.se/~bf/co5bold_main.html</a></td>
<td>Bernd Freytag</td>
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<td>yes/non-grey</td>
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<td>Alexander Vögler</td>
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<td>A Numerical Tool for Astrophysical REsearch</td>
<td><a href="http://arxiv.org/abs/0905.0177">http://arxiv.org/abs/0905.0177</a></td>
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<td>MPI; OpenMP</td>
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<td>Features various high-resolution schemes</td>
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<td>Conservation Law Package</td>
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<td>Randall J. LeVeque</td>
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Computer Codes (cont.): example CO$^5$BOLD code

CO$^5$BOLD stands for CONservative COde for the COmputation of COMpressible CONvection in a BOx of L Dimensions with L=2,3.

CO$^5$BOLD is designed for simulating hydrodynamics and radiative transfer in the outer and inner layers of stars. Additionally, it can treat magnetohydrodynamics, non-equilibrium chemical reaction networks, dynamic hydrogen ionization, and dust formation in stellar atmospheres.
Application examples of CO$^5$BOLD  
(Courtesy Sven Wedemeyer-Böhm)
Simulation of solar granulation with CO\textsubscript{5}BOLD. 400 \times 400 \times 165 grid cells, 11.2 \times 11.2 \text{Mm}, Mean contrast at $\lambda \approx 620 \text{nm}$ is 16.65%.

Courtesy *M. Steffen, AIP*

Simulation of a red supergiant with CO\textsubscript{5}BOLD. $235^3$ grid cells, $m_{\text{star}} = 12m_\odot$, $T_{\text{eff}} = 3436 \text{K}$, $R_{\text{star}} = 875R_\odot$

Courtesy *Bernd Freytag*
Two-dimensional radiation-hydrodynamic simulation of surface convection including the chromospheric layer. The dimensions of the computational domain are: Width, 5600 km; Height above the surface of $\tau = 1$, 1700 km; Depth below this surface level: 1400 km.

Computer Codes (cont.): example CO\textsuperscript{5}BOLD code

CO\textsuperscript{5}BOLD works with

- Cartesian (non-equidistant) grids,
- realistic equation of state,
- non-local, multidimensional radiation transport,
- realistic opacities, opacity binning
- various boundary conditions

CO\textsuperscript{5}BOLD is programmed with

- FORTRAN 90,
- OpenMP directives,

The manual for CO\textsuperscript{5}BOLD can be found under

http://www.astro.uu.se/~bf/co5bold_main.html

Just type CO5BOLD in Google.
11 Equations and boundary conditions

The three-dimensional computational domain encompasses the integral layers from the upper convection zone to the middle chromosphere.

With $120^3$ grid cells, the spatial resolution in the horizontal direction is 40 km, while in the vertical direction it is 20 km throughout the photosphere and chromosphere increasing to 50 km through the convection-zone layer.
The ideal MHD-equations can be written in conservative form as:

$$\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{F} = S,$$

where the vector of conserved variables $\mathbf{U}$, the source term $S$ due to gravity and radiation, and the flux tensor $\mathbf{F}$ are

$$\mathbf{U} = (\rho, \rho \mathbf{v}, \mathbf{B}, E), \quad S = (0, \rho g, 0, \rho g \cdot \mathbf{v} + q_{\text{rad}}),$$

$$\mathbf{F} = \begin{pmatrix}
\rho \mathbf{v} \\
\rho \mathbf{v} \mathbf{v} + \left(p + \frac{\mathbf{B} \cdot \mathbf{B}}{8\pi}\right) \mathbf{I} - \frac{\mathbf{B} \mathbf{B}}{4\pi} \\
\mathbf{v} \mathbf{B} - \mathbf{B} \mathbf{v} \\
\left(E + p + \frac{\mathbf{B} \cdot \mathbf{B}}{8\pi}\right) \mathbf{v} - \frac{1}{4\pi} (\mathbf{v} \cdot \mathbf{B}) \mathbf{B}
\end{pmatrix}.$$

The tensor product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is the tensor $\mathbf{a} \mathbf{b} = \mathbf{C}$ with elements $c_{mn} = a_m b_n$. 
The total energy $E$ is given by

$$E = \rho \epsilon + \rho \frac{v \cdot v}{2} + \frac{B \cdot B}{8\pi},$$

where $\epsilon$ is the thermal energy per unit mass. The additional solenoidality constraint,

$$\nabla \cdot B = 0,$$

must also be fulfilled. The MHD equations must be closed by an equation of state which gives the gas pressure as a function of the density and the thermal energy per unit mass

$$p = p(\rho, \epsilon),$$

usually available to the program in tabulated form. The radiative source term is given by

$$q_{rad} = 4\pi \rho \int \kappa_\nu (J_\nu - B_\nu) d\nu,$$

$$J_\nu(r) = \frac{1}{4\pi} \oint I_\nu(r, n) d\Omega,$$

$$I(r, n) = I_0 e^{-\tau_0} + \int_0^{\tau_0} \left( \frac{\sigma}{\pi} T^4(\tau) \right) e^{-\tau} d\tau.$$
Typical boundary conditions for the thermal variables and velocities

\[ \frac{\partial v_{x,y,z}}{\partial z} = 0 \quad (\text{or} \quad v_z = 0) ; \quad \lim_{t \to \infty} \epsilon = \epsilon_0 \]

\[ \frac{\partial v_{x,y}}{\partial z} = 0 ; \quad \int \rho v_z \, d\sigma = 0 ; \quad \text{outflow:} \quad \frac{\partial s}{\partial z} = 0 \]

\[ \text{inflow:} \quad s = s_0 \]

*Periodic lateral boundary conditions* in all variables. *Open bottom boundary* in the sense that the fluid can freely flow in and out of the computational domain under the condition of vanishing total mass flux.

Reflecting (closed) top boundary or open (transmitting) top boundary.
Boundary conditions for the magnetic field:

\[ B_{x,y} = 0 ; \quad \frac{\partial B_z}{\partial z} = 0 \]

\[ \frac{\partial B_{x,y,z}}{\partial z} = 0 \]

inflow: \( B_y = B_z = 0, B_x = \text{const.} \)

outflow: \( \frac{\partial B_{x,y,z}}{\partial z} = 0 \)
The radiative source term is given by

\[ q_{\text{rad}} = -\nabla \cdot F_{\text{rad}} = 4\pi \rho \int \kappa_\nu (J_\nu - B_\nu) d\nu , \]

\[ J_\nu (r) = \frac{1}{4\pi} \oint I_\nu (r, n) d\Omega , \quad I(r, n) = I_0 e^{-\tau} + \int_0^{\tau_0} \left( \frac{\sigma}{\pi} T^4(\tau) \right) e^{-\tau} d\tau \]

\( \kappa_\nu \): opacity per unit mass \([\text{cm}^2 \text{g}^{-1}]\)

\( \tau \): optical distance to \( r \)
Radiation transfer (cont.)

The (magneto-)hydrodynamics step (advection step) is done independently of the radiative transfer step by operator splitting. The radiative transfer step consists of an energy update step.

Radiative transfer scheme:

- Formal solution of the one-dimensional radiation transfer equation for ‘long rays’. Typically 6 angles in altitude ($\theta$ direction) and 4 angles in azimuth ($\varphi$ direction)
- Realistic (tabulated) opacities
- Grey (one representative frequency point) or frequency dependent treatment with multi-group method (typically 5 opacity bands)
- Strict LTE (no scattering, radiation pressure ignored). ⇒ All rays are independent of each other lending itself to good parallelization
Radiation transfer (cont.)

1. Interpolation from HD grid to RT ray system

HD grid: $\rho$, $e \xrightarrow{\text{EOS}} p, T \rightarrow$ source function $S$, opacity $\rho\kappa$

$\rightarrow$ interpolation (linear) $\rightarrow$ RT Rays system: $S$, $\rho\kappa$

(no velocity needed)
Radiation transfer (cont.)

2. Solution of transfer equation along rays

Ray system: \( \rho \kappa \rightarrow \tau, S(\tau) \)

\[
\frac{\partial^2 y_\nu}{\partial \tau^2} = y_\nu - \frac{\partial^2 S_\nu}{\partial \tau^2}; \quad y_\nu = \frac{1}{2} \left( I_\nu^+ + I_\nu^- \right) - S_\nu
\]

Solution using the Fautrier scheme

Boundary conditions:
Top(\( \tau > 0 \)): incident intensity according to \( T(\tau = 0) = T_{\text{surf}} \)
Bottom: \( (u - S) = 0 \)  or specified flux \( \partial u / \partial \tau = f(T_{\text{eff}}) \)

\( \Rightarrow (u - S) \) along ray at each depth point
3. Back-interpolation from RT ray system to HD grid

RT Ray system: \( \rho \kappa (u - S) \rightarrow \) flux conservative back-interpolation

\rightarrow HD grid: \( \rho \kappa (u - S) \)
4. Angle and frequency integration on HD grid

Lobatto or Gauss quadrature formula for \( \theta \)-integration

1 vertical and \( n \) inclined rays

Simple \( \varphi \)-integration

\( \phi = 0^\circ, 90^\circ, 180^\circ, 270^\circ \) (fixed for 3-D)
Radiation transfer (cont.)

5. Energy update

Summation over $\theta$, $\varphi$, and frequency:

$$Q_{\text{rad}} = 4\pi \int_0^\infty \rho \kappa_\nu (J_\nu - S_\nu) \, d\nu = \sum_{k=1}^{N_{\text{bin}}} \sum_{j=1}^{N_\varphi} \sum_{i=1}^{N_\theta} w_{\varphi,j} w_{\theta,i} \, q(\theta_i, \varphi_j, b_k)$$

where $q(\theta_i, \varphi_j, b_k) = \rho \kappa (u - S)(\theta_i, \varphi_j, b_k)$.

Energy update:

$$e(t + \Delta t) = e(t) + \Delta t \frac{Q_{\text{rad}}}{\rho}$$

Radiative flux:

$$\int_{z_0}^{z_1} \langle Q_{\text{rad}}(x, y, z) \rangle_{x,y} \, dz = \langle F_{\text{rad}}(x, y, z_1) \rangle_{x,y} - \langle F_{\text{rad}}(x, y, z_0) \rangle_{x,y}$$
Radiation transfer (cont.)

MSrad3D control parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>opta file</td>
<td>name of opacity table</td>
<td>g2vb.opta</td>
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<tr>
<td>n_radband</td>
<td>gray or multi group RT (1,2,3,4)</td>
<td>2</td>
</tr>
<tr>
<td>c_radhtautop</td>
<td>opacity scale height at upper bndr</td>
<td>60.0E+05</td>
</tr>
<tr>
<td>c_tsurf</td>
<td>$T_{surf} = c_{tsurf} T_{eff}$</td>
<td>0.73</td>
</tr>
<tr>
<td>n_radthickpoint</td>
<td>number of layers with diffusion RT</td>
<td>48</td>
</tr>
<tr>
<td>n_radtheta</td>
<td>number of $\theta$ angles (0...4)</td>
<td>2</td>
</tr>
<tr>
<td>n_radphi</td>
<td>number of $\varphi$ angles (0...6 in 2-D)</td>
<td>2</td>
</tr>
<tr>
<td>n_radsubray</td>
<td>number of rays per $\Delta x$ of DS-grid</td>
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</tr>
<tr>
<td>n_radtaurefine</td>
<td>number of RT levels per $\Delta z$ of HD grid</td>
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</tr>
<tr>
<td>radraybase</td>
<td>quadrature method for $\theta$-integration</td>
<td>lobatto</td>
</tr>
<tr>
<td>bottom_bound</td>
<td>lower bnd condition for RT</td>
<td>inoutflow</td>
</tr>
</tbody>
</table>
MSrad3D control parameter $c_{\text{radhtautop}}$ and $c_{\text{tsurf}}$

\[ I_{1}^{-} = S_{0}\left\{ (1 - f)/\tau_{1} - f \right\} + S_{1}\left\{ 1 - (1 - f)/\tau_{1} \right\} , \quad f = e^{-\tau_{1}} \]

\[ I_{0}^{+} = I_{1}^{+}e^{-\tau_{1}} + S_{1}\left\{ (1 - f)/\tau_{1} - f \right\} + S_{0}\left\{ 1 - (1 - f)/\tau_{1} \right\} \]
Radiation transfer (cont.)

MSrad3D control parameter $n_{radthickpoints}$

$n_{radthickpoints} = 3$

RT ray system

RT diffusion approximation
MSrad3D control parameter \( c_{\text{radsubray}} \)

\[ n_{\text{radsubray}} = 3 \]
Radiation transfer (cont.)

MSrad3D control parameter \( n_{\text{radtaurefine}} \)

\( n_{\text{radtaurefine}} = 3 \)
Radiation transfer (cont.)

MSrad3D control parameter *bottom_bound* The radiation transfer equation is solved using a modified Fautrier scheme.

\[
\frac{\partial^2 y_\nu}{\partial \tau_\nu^2} = y_\nu - \frac{\partial^2 S_\nu}{\partial \tau_\nu^2}; \quad y_\nu = \frac{1}{2}(I^+_\nu + I^-_\nu) - S_\nu \overbrace{u_\nu}^\text{boundary}
\]

Boundary conditions:

*bottom_bound* = inoutflow \(\Rightarrow\) \(y_\nu = (y_\nu - S_\nu) = 0 \quad (\nabla F_{\text{rad}} = 0)\)

else \(\Rightarrow\) \(\partial u_\nu / \partial \tau = (3/4)F_{\text{rad}}/\pi w_\nu \cos(\theta)\)
12.1 Multi-group radiation transfer  

\[ q_{\text{rad}} = - \nabla \cdot F_{\text{rad}} = 4\pi \rho \int \kappa_{\lambda} (J_{\lambda} - B_{\lambda}) \, d\lambda , \]

\[ \int \kappa_{\lambda}(J_{\lambda} - B_{\lambda}) \, d\lambda = \sum_j \kappa_{\lambda_j}(J_{\lambda_j} - B_{\lambda_j}) \, w_{\lambda_j} \]

\[ = \sum_i \sum_j \kappa_{\lambda_j}(J_{\lambda_j} - B_{\lambda_j}) \, w_{\lambda_j} \]

\[ = \sum_i \sum_j \kappa_{\lambda_j}( \Lambda_{\lambda_j}(B_{\lambda_j}) - B_{\lambda_j}) \, w_{\lambda_j} \]

\[ \approx \sum_i \kappa_i(\Lambda_i - 1)(\sum_j B_{\lambda_j} \, w_{\lambda_j}) \]

\[ \approx \sum_i \kappa_i(\Lambda_i - 1)(B_i \, w_i) \equiv \sum_i \kappa_i(J_i - B_i)w_i \]
Strategy for opacity binning:

- concentrate on radiative transfer in vertical direction,

- group together frequencies with as similar a $\tau^s_\nu$-relationship as possible, so that $\Lambda_{\lambda_j(i)}$ is very similar $\forall j$ of a given bin $i$,

- choose clever averaging procedure for $\kappa_\nu$, (Rosseland averages for $\tau_i > 1$, Planck averages for $\tau_i < 1$).
Multi-group radiation transfer (cont.)

The art of opacity binning: Constructing the bands (H.-G. Ludwig, Paris Obs.)

![Diagram showing opacity binning](image)

- **Band 1**: \( \tau_R(\tau_\nu = 1) > \tau^1_R \)  
  - "continuum"
- **Band 2**: \( \tau^1_R \geq \tau_R(\tau_\nu = 1) > \tau^2_R \)  
  - "weak lines"
- **Band 3**: \( \tau^2_R \geq \tau_R(\tau_\nu = 1) > \tau^3_R \)  
  - "medium strong lines"
- **Band 4**: \( \tau^3_R \geq \tau_R(\tau_\nu = 1) \)  
  - "strong lines"
Multi-group radiation transfer (cont.)

Testing the OBM. Integrated radiative flux

Reference atmosphere: Radiative Flux

![Graph showing the reference atmosphere radiative flux with different resolution and binning methods]
Multi-group radiation transfer (cont.)

Intensity maps for different opacity bins

Notice that bin 3 to 5 show “inverse granulation” as their opacities represent medium to strong line cores.
Multi-group radiation transfer (cont.)

Mean enthalpy flux, kinetic energy flux, and radiative energy flux as a function of height.
Multi-group radiation transfer (cont.)

Radiative cooling (bright) and heating (dark), $Q_{\text{rad}}$

Note that there is slight radiative heating in the low photosphere due to the “line blanketing”.

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toc   ref
13 Chemical reaction network

For certain applications, e.g., the effect of CO in the solar atmosphere, an optional module for the treatment of a network of chemical reactions was added to the CO$^5$BOLD code. For further details see Wedemeyer-Böhm et al. (2005), A&A 438, 1043 and Wedemeyer-Böhm & Steffen (2007), A&A 462, L31.

The operator splitting method is used in order to account for the time evolution of chemical species. In a first step the chemical species are advected together with all the other hydrodynamic quantities:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{v}) = 0,$$

where $n_i$ is the number density of a chemical species and $\mathbf{v}$ the velocity of the hydrodynamical flow.
In a second step (between the hydro step and the radiation-transfer step), the change in number density due to chemical reactions is accounted for:

\[
\left( \frac{\partial n_i}{\partial t} \right)_{\text{chem}} = -n_i \sum_j k_{2,ij} n_j \\
+ \sum_j \sum_l k_{2,jl} n_j n_l \\
- n_j \sum_i \sum_l k_{3,ijl} n_j n_l \\
+ \sum_j \sum_l \sum_m k_{3,jlm} n_j n_l n_m ,
\]

where \( n_i \) is the number densities of species \( i \), which decreases or increases due to two-body reactions with rates \( k_{2,ij} \) and \( k_{2,jl} \), respectively. Three-body reactions are analogously accounted for by the third and fourth term with rates \( k_{3,ijl} \) and \( k_{3,jlm} \). It results in a (stiff!) system of ordinary differential equations.
Chemical reaction network (cont.)

The rates have the basic form

\[ k = \alpha T^{\beta} e^{-\gamma/T}, \]

where \( T_{300} = T/300 \text{K} \). For catalytic reactions the number density of a representative metal \( n_M \) enters: The rates have the basic form

\[ k = n_M \alpha T^{\beta} e^{-\gamma/T}. \]

The coefficients \( \alpha, \beta, \text{ and } \gamma \) are compiled in tables, e.g., in Wedemeyer-Böhm et al. (2005), A&A 438, 1043.
Chemical reaction network:
7 chemical species, H, H₂, C, O, CO, CH, OH, plus a representative metal M
27 chemical reactions
Chemical reaction network (cont.)

Radiative cooling via CO lines:

- Two opacity bands:
  1.) *continuum band* with Rosseland mean opacity $\kappa_R$ without infrared.
  2.) *infrared band* at 4.7 $\mu$m with Rosseland mean opacity plus CO line opacity, $\kappa_R + \kappa_{CO}$.

- CO opacity calculated from (time dependent) CO number density.

Application examples:

- *movie* of CO number density in two-dimensional hydrodynamic solar convection.
- *animation* of “CO clouds” from a three-dimensional simulation.
14 Non-equilibrium Hydrogen ionization in CO$^5$BOLD

The assumption of strict LTE and the “grey” approximation may be tenable when studying the dynamics of magnetic fields in the chromosphere – it is certainly not adequate for quantitative spectroscopy.

Under the condition of the solar chromosphere the assumption of LTE (local thermodynamic equilibrium) is not valid. Even the assumption of statistical equilibrium in the rate equations is not valid. Kneer (1980) showed that the relaxation timescale for the ionization of hydrogen varies from 100 s to 1000 s in the middle to upper chromosphere.

In order to compute the \textit{time dependent hydrogen ionization} in a three-dimensional environment, simplifications are needed. We employ the \textit{method of fixed radiative rates}. We solve the time-dependent rate equations

\[
\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{v}) = \sum_{j \neq i} n_j P_{ji} - n_i \sum_{j \neq i} P_{ij}
\]

\[
P_{ij} = C_{ij} + R_{ij}.
\]
Non-equilibrium Hydrogen ionization in CO$^5$BOLD (cont.)

In the method of fixed radiative rates we assume that the radiation field in each transition, both, bound-bound and bound-free, can be described by a formal radiation temperature:

$$J_\nu = \frac{2\hbar \nu^3}{c^2} \frac{1}{e^{\hbar \nu / kT_{\text{rad}}} - 1}$$

Thus, we obtain the *fixed radiative rates* for bound-bound transitions

$$R_{lu} = B_{lu} J_{\nu_0} = \frac{4\pi^2 e^2}{\hbar \nu_0 m_e c} f_{lu} \frac{2\hbar \nu_0^3}{c^2} \frac{e^{\hbar \nu_0 / kT_{\text{rad}}} - 1}{e^{\hbar \nu_0 / kT_{\text{rad}}} - 1}$$

$$R_{ul} = A_{ul} + B_{ul} J_{\nu_0} = \frac{g_l}{g_u} e^{\hbar \nu_0 / kT_{\text{rad}}} R_{lu}$$
The hydrogen bound-free excitations have a Kramer’s absorption cross section:

$$\sigma_{ic}(\nu) = \alpha_0 \left(\frac{\nu_0}{\nu}\right)^3, \nu > \nu_0,$$

where $\alpha_0$ is the absorption cross-section at the edge frequency $\nu_0$. In this case the radiative rate coefficients are

$$R_{ic} = 4\pi \int_{\nu_0}^{\infty} \frac{\sigma_{ic}(\nu)}{h\nu} J_\nu d\nu = \frac{8\pi}{c^2} \alpha_0 \nu_0^3 \int_{\nu_0}^{\infty} \frac{1}{\nu} \frac{1}{e^{h\nu/kT_{rad}} - 1} d\nu$$

$$= \frac{8\pi}{c^2} \alpha_0 \nu_0^3 \sum_{n=1}^{\infty} E_1 \left[ n \frac{h\nu_0}{kT_{rad}} \right] , \quad E_1 \text{ being the first exponential integral}$$

$$R_{ci} = 4\pi \left[ \frac{n_i}{n_c} \right]_{LTE} \int_{\nu_0}^{\infty} \frac{\sigma_{ic}(\nu)}{h\nu} \left( \frac{2h\nu^3}{c^2} + J_\nu \right) e^{-h\nu/kT_e} d\nu$$

$$= \frac{8\pi}{c^2} \alpha_0 \nu_0^3 \left[ \frac{n_i}{n_c} \right]_{LTE} \sum_{n=1}^{\infty} E_1 \left[ \left( n \frac{T_e}{T_{rad}} + 1 \right) \frac{h\nu_0}{kT_e} \right].$$
Non-equilibrium Hydrogen ionization in $\text{CO}_5^{5}$BOLD (cont.)

Effect of dynamic H-ionization in the upper part of a 2-D simulation. *Left column:* LTE ionization degree and electron density. *Right column:* Corresponding time-dependent *NLTE* quantities. Bottom left: Gas temperature, which is the same for the LTE and the time-dependent case. *Leenaarts & Wedemeyer-Böhm 2006*
References


References (cont.)


Part IV: Aspects of computational astrophysics
15 Role of computer simulations

How can astrophysicists

- inform about the first milliseconds of a core collapse supernova,
- know about the past million years of dynamical evolution of a present day galaxy,
- know about the structure formation of the early universe,
- talk about the state of the plasma of stellar interiors as if they had it examined in the laboratory?

Answer: With the help of computational astrophysics!
The antenna nebula NGC 4038/4039 evolved from a collision of two similarly sized spiral nebulae. *Left:* Observed present state. *Right:* Present state from a computer simulation of the complete collision (www.ifa.hawaii.edu/~barnes).

Four instants in the formation of a neutron star in the course of a supernova explosion. From the top right panel counterclockwise 3 milliseconds apart in a radial region from $R = 15\text{ km}$ to $R = 155\text{ km}$ (www.MPA-Garching.MPG.de).
Role of computer simulations (cont.)

_Historical Perspective:_

- 1950’s and 1960’s: Stellar evolution calculations (Martin Schwarzschild in the U.S. and Rudolph Kippenhahn in Göttingen, Germany). At that time *computers were viewed as tools for the numerical integration* rather than as a tool for experimentation.

- 1960’s: N-body stellar dynamics simulations (e.g. tidal interaction of galaxies) and hydrodynamical systems (e.g. core collapse supernovae). Notion of *computational astrophysics as experimental astronomy*. These simulations are generally _motivated by the question “What happens if?”_ more so than “What is the solution to these equations?”.

Computational astrophysics is the experimentation with astrophysical objects in a virtual (numerical) laboratory, comparable to the manipulation with real probes in classical physics experiments.
Role of Computational astrophysics:

Adapted from M. Norman (1997)
Role of computer simulations (cont.)

*Interaction theory ↔ computational astrophysics*

- Theory provides the mathematical formulation for the simulation.

- Analytical properties of the solution can be incorporated into the numerical algorithm (e.g., conservation laws, Rankine-Hugoniot relations, etc.).

- Analytical solutions provide *test problems* for validation.

- Complex simulation results can post facto be reduced to *analytical toy models*, which nonetheless capture the essential physics (to become enshrined in astronomy textbooks).

- Simulations provide realizations of the theoretical formulation. They may hint at missing ‘physics’ in the formulation and build *physical intuition* regarding the phenomena embodied in the governing equations.

- *Numerical experiments* aim at revealing the essential physics of an astrophysical process.
Interaction observation $\leftrightarrow$ computational astrophysics

- Observations provide the final validation of the simulation.
- Postdiction of available observational data in the early phase.
- Prediction of observational data with more mature simulations.

For the comparison of simulation results with observations it is essential that observable quantities, for short observables, are computed, i.e., synthesized from the simulation data. Results from such “numerical” or “virtual observations” are sometimes called “synthetic data”.

The generation of synthetic observables from the simulation data is often as time consuming as the simulation itself.
Role of computer simulations (cont.)

Progress in computational astrophysics:

Adapted from M. Norman (1997)
References


Part V: MHD simulations: Case studies
Case study I: Magnetic fields of the quiet Sun
Continuum at 395 nm with the VTT and KAOS at Tenerife

G-band bright points, Muller, 1985.
Hinode (Solar-B) launched on 22 September 2006. The Solar Optical Telescope (SOT) has an aperture of 50 cm featuring an image stabilization system consisting of a piezo-driven tip-tilt mirror. The Spectral-polarimeter (SP) generates Stokes $IQUV$ spectral images.

http://solar-b.nao.ac.jp
Case study I: Magnetic fields of the quiet Sun (cont.)

Continuum intensity at 630 nm over a field of view of $302'' \times 162''$. From *Lites et. al. 2008, ApJ 672, 1237*
Case study I: Magnetic fields of the quiet Sun (cont.)

Apparent vertical magnetic flux density, $B_{\text{app}}^L$, of the quiet Sun over a field of view of $302'' \times 162''$. The grey scale saturates at $\pm 50 \text{ Mx cm}^{-2}$. 2048 steps to 5 s.

$\langle |B_{\text{app}}^L| \rangle = 11.7 \text{ Mx cm}^{-2}$. From Lites et. al. 2008, ApJ 672, 1237
Apparent horizontal magnetic flux density, $B_{\text{app}}^T$, of the quiet Sun over a field of view of $302'' \times 162''$. The grey scale saturates at $\pm 200 \text{ Mx cm}^{-2}$. 2048 steps to 5 s.

$\langle B_{\text{app}}^T \rangle = 60.0 \text{ Mx cm}^{-2}$. From Lites et. al. 08
Deep mode *Stokes spectra* with an integration time of 67.2 s and a rms polarization in the continuum of $3 \times 10^{-4}$. From a 2-hour time series Lites et al. obtain mean apparent longitudinal and transversal field strengths of $\langle B^L_{\text{app}} \rangle = 11.0 \, \text{Mx cm}^{-2}$ and $\langle B^T_{\text{app}} \rangle = 55.3 \, \text{Mx cm}^{-2}$. From *Lites et al. 08*
**Case study I: Magnetic fields of the quiet Sun (cont.)**

*Red and green:* contours of $B_{\text{app}}^L = 24 \text{ Mx cm}^{-2}$, respectively positive and negative. *Yellow:* contours of $B_{\text{app}}^L = 100 \text{ Mx cm}^{-2}$. *Blue* contours correspond to $B_{\text{app}}^T = 122 \text{ Mx cm}^{-2}$. Horizontal flux preferentially occurs at locations between lanes and granule centers. From *Lites et. al. 08*
Case study I: Magnetic fields of the quiet Sun (cont.)

A predominance of horizontally directed magnetic fields in the quiet Sun was also reported by Orozco Suárez et al. 07 from HINODE measurements and by Harvey et al. 07 from center-to-limb measurements with GONG and SOLIS.

![Probability density of the magnetic field inclination in the inter-network. From Orozco Suárez et al. 07.](image)

Ishikawa et. al. 08 detected transient horizontal magnetic fields in plage regions with SOT/HINODE

Previously, Meunier et al. 1998 and Martinez Pillet et al. 97 reported observations of weak and strong horizontal field in quiet Sun regions.
Case study I: Magnetic fields of the quiet Sun (cont.)

**Questions:**

- Do simulations of the surface layers of the Sun intrinsically produce horizontal magnetic fields?
- If yes, how do they originate?
- How does the polarimetric signal from simulations compare to measurements?


Grossmann-Doerth et al. 1998 noted: “we find in all simulations also strong horizontal fields above convective upflows”
Typical size of a three-dimensional computational box (left) on scale with the convection zone boundaries (right)
Numerical simulation of near surface magnetoconvection (cont.)

Different initial states and boundary conditions for the magnetic field

Initial homogeneous, vertical, unipolar $B$-field of 10 G.

Fluid that enters the simulation domain from below carries horizontal magnetic field of $B_x = 20$ G.

$B_{x,y} = 0; \quad \partial B_z / \partial z = 0$

$\partial B_{x,y,z} / \partial z = 0$

→ more
Numerical simulation of near surface magnetoconvection (cont.)

Vertical cross sections through 3-D simulation domain

Colors indicate $0 \leq \log |B| \leq 3.0$

Colors indicate $0.5 \leq \log |B| \leq 2.5$
Numerical simulation of near surface magnetoconvection (cont.)

Horizontally and temporally averaged absolute vertical and horizontal magnetic flux density as a function of height for both runs.

\[
\langle B_{\text{hor}} \rangle = \langle \sqrt{B_x^2 + B_y^2} \rangle
\]

run v10:
\[
\langle B_{\text{hor}} \rangle / \langle |B_{\text{ver}}| \rangle (500 \text{ km}) = 2.5
\]

run h20:
\[
\langle B_{\text{hor}} \rangle / \langle |B_{\text{ver}}| \rangle (420 \text{ km}) = 5.6
\]
Numerical simulation of near surface magnetoconvection (cont.)

$\langle B_{\text{hor}} \rangle$ (———) and $\langle B_{\text{ver}} \rangle$ (– – – – –) as a function of height $z$ for run h20 (heavy) and run v10 (thin).
From Steiner et al. 2008

$\langle B_x \rangle$ (− · − · − · − ), $\langle B_y \rangle$ (· . . . . . ), and $\langle B_{\text{ver}} \rangle$ (− − − − −) as a function of $\log \tau_{630 \text{ nm}}$.
From Schüssler & Vögler 2008
Numerical simulation of near surface magnetoconvection (cont.)

Vertical section through computational domain...

... shows horizontal sheets of enhanced magnetic field strength in the upper photosphere — \textit{the seething magnetic field}. \rightarrow T movie
Numerical simulation of near surface magnetoconvection (cont.)

Snapshot of $B_{\text{hor}}$, $B_{\text{ver}}$, and the continuum intensity at 630 nm from run h20 in the horizontal section of $\langle \tau_{500\,\text{nm}} \rangle = 1$.

- $B_{\text{hor}}$ area fraction with $B_{\text{hor}} > 5$ mT = 17%
- $B_{\text{ver}}$ area fraction with $B_{\text{ver}} > 5$ mT = 2.2%
- $I_{630\,\text{nm}}$

Movie
We synthesized the Stokes profiles of both 630 nm Fe I spectral lines observed by the Hinode SP with a spectral sampling of 2 pm.

We then compute

\[ V_{\text{tot}} = \frac{\int_{\lambda_b}^{\lambda_0} V(\lambda) \, d\lambda - \int_{\lambda_0}^{\lambda_r} V(\lambda) \, d\lambda}{I_c}, \]

and

\[ Q_{\text{tot}} = \frac{\int Q(\lambda) Q_{\text{mask}}(\lambda) \, d\lambda}{I_c}, \]

We subject these quantities to exactly the same calibration procedure for conversion to apparent flux density as was done with the real data by Lites et al. 08.
Polarimetry (cont.)

From the two simulation runs, we synthesized the Stokes profiles of both 630 nm Fe I spectral lines observed by the Hinode SP. Profiles were computed with the radiative transfer code SIR along vertical lines of sight (disk center) with a spectral sampling of 2 pm.

\[ I_{630 \text{ nm}} \quad \text{and} \quad V_{\text{tot} 630 \text{ nm}} \]
Polarimetry (cont.)

Synthetic continuum intensity at 630 nm and $V_{\text{tot}}$ from a simulation with box size $9.6 \times 9.6$ Mm, corresponding to $13'' \times 13''$. 

$I_{630 \text{ nm}}$  \hspace{1cm} $V_{\text{tot} 630 \text{ nm}}$
Polarimetry (cont.)

Calibration curve from Lites et al. 07 derived from a Milne-Eddington atmosphere with a homogeneous horizontal magnetic field for $Q_{\text{tot}}$ and a magnetic field inclined by $45^\circ$ for $V_{\text{tot}}$. 
Lites et al. (2007) found from the deep mode series

\[
\frac{\langle B^{T}_{\text{app}} \rangle}{\langle B^{L}_{\text{app}} \rangle} = \frac{55.3 \text{ Mx cm}^{-2}}{11.0 \text{ Mx cm}^{-2}} \approx 5.
\]

From the synthesized Stokes profiles and application of the SOT-PSF we find

\[
\frac{\langle B^{T}_{\text{app}} \rangle}{\langle B^{L}_{\text{app}} \rangle} = \begin{cases} 
10.4 \text{ G}/6.6 \text{ G} = 1.6 & \text{for run } v10 \\
21.5 \text{ G}/5.0 \text{ G} = 4.3 & \text{for run } h20
\end{cases}.
\]

without the PSF we got

\[
\frac{\langle B^{T}_{\text{app}} \rangle}{\langle B^{L}_{\text{app}} \rangle} = \begin{cases} 
11.5 \text{ G}/7.5 \text{ G} = 1.5 & \text{for run } v10 \\
24.8 \text{ G}/8.8 \text{ G} = 2.8 & \text{for run } h20
\end{cases}.
\]
Polarimetry (cont.)

The vertical field component is more subject to apparent flux cancellation than the horizontal component, because ....

\[ B_{\text{hor}} \]

..... the vertical field component has smaller scales and higher intermittency than the horizontal component.
Polarimetry (cont.)

Probability density functions of the magnetic field inclination from observations of Orozco Suárez et al. (2007) and simulations.

Solid and dashed PDFs represent all pixels in the FOV and the IN regions, respectively. Dot-dashed curve shows PDFs from magnetoconvection simulations with a mean flux density of 10 Mx cm$^{-2}$ from Vögler et al. (2005).

PDF of inclination angle for simulation runs h20 and v10 of Steiner et al. (2008).
Polarimetry (cont.)

Center-to-limb variation

Vertical field dominates in the low photosphere
Horizontal field dominates in the upper photosphere

Horizontal field dominates throughout the photosphere
The horizontal field can be considered a consequence of the *flux expulsion process* (Weiss, 1966; Galloway & Weiss, 1981): in the same way as magnetic flux is expelled from the granular interior to the intergranular lanes, it also gets pushed to the middle and upper photosphere by overshooting convection, where it tends to form a layer of horizontal field.

From *Galloway & Weiss, 1981*
Flux expulsion in a close-up from a MHD simulation by Schaffenberger et al. (2005)
The dominance of the horizontal field “results from the intermittent nature of the dynamo field with polarity mixing on small scales in the surface layers”.

From Schüssler & Vögler 2008
Detached horizontal field as a consequence of magnetic reconnection
20 Horizontal magnetic fields: Poynting flux

Equation for the total energy:

$$\frac{\partial e}{\partial t} + \nabla \left[ (h + \frac{1}{2} v^2) \rho v + S \right] - \mathbf{g} \cdot \mathbf{v} = 0,$$

where

$$e = \rho \epsilon + \frac{1}{2} \rho v^2 + \frac{B^2}{2 \mu}, \quad h = \epsilon + \frac{p}{\rho},$$

and

$$S = \frac{1}{4\pi} (\mathbf{B} \times (\mathbf{v} \times \mathbf{B}))$$

Magnetic energy equation:

$$\frac{\partial}{\partial t} \left( \frac{B^2}{8\pi} \right) = - \nabla \cdot (\mathbf{E} \times \mathbf{B}) - \mathbf{u} \cdot (\mathbf{j} \times \mathbf{B}) - Q_{\text{res}}$$

Poynting flux  Lorentz work
Horizontal magnetic fields: Poynting flux (cont.)

Vertically directed Poynting flux, $\langle S_z \rangle$, $\langle B_{\text{hor}} \rangle$, and $\langle |B_z| \rangle$ as a function of time and height in the atmosphere.

$$S = \frac{1}{4\pi} (\mathbf{B} \times (\mathbf{v} \times \mathbf{B}))$$


The surface of optical depth unity is a separatrix for the vertically directed Poynting flux.
Vertically directed Poynting flux, $\langle S_z \rangle$, as a function of height in the atmosphere.

The temporal average of $\langle S_z \rangle$ is maximal $7.4 \times 10^2$ Wm$^{-2}$ (at 200 km) and minimal $-5.2 \times 10^4$ Wm$^{-2}$ (at $-800$ km). For comparison: the chromospheric radiative energy loss is about $4.3 \times 10^3$ Wm$^{-2}$. 
Horizontal magnetic fields: Poynting flux (cont.)

Logarithmic current density, $\log |j|$, in a vertical cross section (top panel) and in four horizontal cross sections in a depth of 1180 km below, and at heights of 90 km, 610 km, and 1310 km above the average height of optical depth unity from left to right, respectively. The arrows in the top panel indicate the magnetic field strength and direction.

Top: Logarithm of the magnetic field strength. Bottom: Logarithm of the current density.

Top: Vertical cross sections of $|B|$ and the velocity vector projected onto the plane.

Bottom: Horizontal cross sections at $z = 0$, showing $B_\parallel$ (gray scale) and $B_z$ (contours), and the magnetic vectors projected onto the plane.

Case study II: Structure of internetwork magnetic elements

Apparent vertical magnetic flux density $B_{\text{app}}^L$ of the quiet Sun over a field of view of $302'' \times 162''$ observed from the Hinode space observatory. The grey scale saturates at $\pm 50 \text{ Mx cm}^{-2}$. 2048 steps to 5 s.
Stokes-$V$ profiles across a magnetic element of the internetwork from the Hinode data.

\[ \delta A := \frac{A_b - A_r}{A_b + A_r} \]

\[ \text{sign}(\delta A) = -\text{sign}(\frac{d|B|}{d\tau} \cdot \frac{d\nu(\tau)}{d\tau}) \]

Solanki & Pahlke, 1988; Sanchez Almeida et al., 1989
Case study II: Structure of internetwork magnetic elements (cont.)

Columns a-c: observational data obtained with the spectro-polarimeter of Hinode/SOT. Columns d and f: synthetic data from the 3-D MHD simulation. Columns e and g: same as d and f but after application of the SOT-PSF to the synthetic intensity maps. Distance between tick marks is 0.5″.

From Rezaei, Steiner, Wedemeyer-Böhm et al. 2007, A&A 476, L33
Case study II: Structure of internetwork magnetic elements (cont.)

Variation in $\delta A$ across magnetic elements from the Hinode data (top row) and the simulation (bottom row).
Case study II: Structure of internetwork magnetic elements (cont.)

Vertical cross section through the simulation box. *Colour* displays the logarithmic magnetic field strength, *arrows* the velocity field, *black contours* the electric current density normal to the plane. The *white vertical lines* indicate ranges of either positive or negative area asymmetry, $\delta A$. 

$$\begin{align*}
\frac{d|B|}{d\tau} < 0 \\
\frac{dv(\tau)}{d\tau} > 0
\end{align*} \Rightarrow \delta A > 0$$
Case study III: Wave propagation in a magnetically structured atmosphere

Time sequence of a two-dimensional simulation of magnetoconvection starting with an initial homogeneous vertical magnetic field of 100 G.

*Left:* Temperature, *Right:* Absolute magnetic field strength. A magnetic flux sheet has formed at $x \approx 4200$ km.
Case study III: Wave propagation in a magnetically structured atmosphere (cont.)

The sequence from \(t = 1200\) s to \(t = 1450\) s is repeated with a plane parallel, oscillatory velocity perturbation at the bottom boundary with an amplitude of 50 m/s and a frequency of 20 mHz. When subtracting the velocity field of the two sequences, the perturbation becomes visible.

*Left:* Magnetic field strength. *Right:* Subtractive velocity field 116 s after starting the perturbation.
Case study III: Wave propagation in a magnetically structured atmosphere (cont.)

Residual velocity amplitude due to an oscillatory velocity perturbation along the bottom

\[ v_z(t) = v_0 \sin(2\pi(t - t_0)\nu) \]

with an amplitude of \( v_0 = 50 \text{ m/s} \) and a frequency of \( \nu_0 = 20 \text{ mHz} \) from \( t = 1200 \text{ s} \) to \( t = 1450 \text{ s} \). Note the fast magnetic wave that gets refracted.

*Left:* Logarithmic magnetic field strength 1368 s after starting with an initial homogeneous vertical field of 100 G. *Right:* Logarithm of thermal to magnetic energy density (plasma-\( \beta \)) together with the contour of \( \beta = 1 \).
Case study III: Wave propagation in a magnetically structured atmosphere (cont.)

Wave travel time vs. canopy height.

Wave travel time across the layer from $z = 200$ km to $z = 420$ km as a function of horizontal distance (thick solid curve). Superposed is the contour of $\beta = 1$ (magnetic and thermal equipartition), for which the height is indicated in the right hand side ordinate (dash-dotted curve). Note that the travel time markedly decreases where the low $\beta$ region intrudes this layer. From Steiner, Vigeesh, Krieger et al. 2007
Case study III: Wave propagation in a magnetically structured atmosphere (cont.)

Finsterle et al. 2004, ApJ 613, L185 suggest to determine the three-dimensional topography of the $\beta = 1$-surface by measuring the travel time of high frequency waves between lines formed below and above this surface. They use a MOTH-MDI combined data set of 17.8 h duration.

Helioseismic mapping of the magnetic canopy in the solar chromosphere
Maps of travel time for 7 mHz waves between the formation layers of (a) Ni and Na, (b) K and Na, and (c) Ni and K. (d) the contemporaneous MDI magnetogram. $\beta \approx 1$ contours at 200 km (white), 420 km (black-white), and 800 km (black) above $\tau_c = 1$.

Case study III: Wave propagation in a magnetically structured atmosphere (cont.)

Time instant of a spherical, fast acoustic wave, initiated by a local pressure perturbation in the convection zone. When the wave encounters the low beta magnetic flux concentration in the photosphere it partially converts into a fast magnetic mode, which shows the typical “fanning out” already encountered in the 2-D simulation. Colors show absolute velocity perturbation. Courtesy Christian Nutto, KIS.
Case study III: Wave propagation in a magnetically structured atmosphere (cont.)

2 kG uniform magnetic field inclined at ±30° to the vertical. The incoming 5 mHz rays have lower turning points at \( z = -5 \) Mm. The horizontal grey line indicates where the sound and Alfvén speeds coincide. The fractional energy remaining in each resulting ray is indicated in grey scales. The dots on the ray paths indicate 1 min group travel time intervals. The thin black curve represents the acoustic ray that would be there in the absence of magnetic field. From Cally (2007) AN 328, 286

Movie top panel
Movie bottom panel
Case study III: Wave propagation in a magnetically structured atmosphere (cont.)

2 kG uniform vertical magnetic field. Here, the 5 mHz frequency is not sufficient to overcome the atmospheric acoustic cutoff (5.2 mHz), and the upgoing slow ray reflects back downward. From Cally (2007) AN 328, 286
Case study III: Wave propagation in a magnetically structured atmosphere (cont.)

Transversal, impulsive excitation at the footpoint of a magnetic flux sheet.

\[ v_x = v_0 \sin(2\pi t / P), \quad P = 24 \text{ s}, \quad v_0 = 750 \text{ ms}^{-1} \]

\[ v_\parallel \text{ after 40 s} \quad v_\perp \text{ after 40 s} \quad \delta T \text{ after 40 s} \]
Case study IV: The restless chromosphere

Simulations show a fast changing pattern of enhanced temperatures in the chromosphere, termed the *fluctosphere*, or *clapotisphere*. It is distinctly different from the pattern of inverse granulation in the middle photosphere, and the granulation itself.

\[ T(z = -200\text{km}) \quad T(z = +200\text{km}) \quad T(z = +1000\text{km}) \]
Case study IV: The restless chromosphere (cont.)

Filtergrams in the infrared line Ca II 854 nm

Wöger et al. 2006

observed in 0.3 Å filtergrams centred at the Ca II K$_{2\nu}$ peak a short-lived pattern with a typical spatial scale of 1.95" and a mean evolution time scale of 53 s.

Courtesy, S. Wedemeyer-Böhm
Case study IV: The restless chromosphere (cont.)

Intensity image at $\lambda = 1$ mm of the “fluctosphere” at different spatial resolutions:

- **a)** 0.06” (size of computational grid cells),
- **b)** 0.3”,
- **c)** 0.6”,
- **d)** 0.9”.

![Intensity image at different spatial resolutions](image)

Case study IV: The restless chromosphere (cont.)

Snapshot of a vertical section showing $\log |B|$ (color coded) and velocity vectors projected on the vertical plane (white arrows). The b/w dashed curve shows optical depth unity and the dot-dashed and solid black contours $\beta = 1$ and 100, respectively.

Case study IV: The restless chromosphere (cont.)

Two instances of shock induced magnetic field compression. Absolute magnetic flux density (colors) with velocity field (arrows), $Mach = 1$-contour (dashed) and $\beta = 1$-contour (white solid).
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Part VI: Future directions
Big: Efforts are underway to increase the simulation box so as to accommodate a supergranulation cell. Recently, Stein et al. carried out a simulation of $48 \times 48 \times 20$ Mm using $500^3$ grid cells. With this simulation they hope to find out more about the origin of supergranulation and to carry out helioseismological experiments.
Simulations at large scales and high resolution (cont.)

**Bigger:** Numerical simulation of a pair of sunspots: Intensity map.

Movie of $B_z$.  

Simulations at large scales and high resolution (cont.)

These simulations suggest a unified physical explanation for umbral dots and the penumbrae in terms of magneto-convection in a magnetic field with varying inclination. A consistent physical picture of all observational characteristics of sunspots and their surroundings is emerging.

(A) $B_z$, (B) inclination angle of $B$, (C) radial outflow velocity (red outflow), (D) vertical velocity.
Simulations at large scales and high resolution (cont.)

**Biggest**: Global simulation of the solar convection zone.

(a,c) Volume renderings of $B_\Phi$ and $B_\gamma$. Red tones indicate prograde fields, and blue tones denote retrograde fields. (b) Selected subvolume of $B$ in the equatorial plane. Typical field strengths are about 1000 G for $B_\gamma$ and 3000 G for $B_\Phi$.

(d) Potential field extrapolation of the radial magnetic field.

**Movie**: Radial magnetic field in a rotating convective spherical shell. Dark tones for the negative polarity and bright tones for the positive polarity.

**Movie**: Radial convective velocity. Blue/black tones for downflows and red/yellow tones for upflows.

*Brun, Miesch & Toomre (2004)*
Simulations at large scales and high resolution (cont.)

“Holistic simulation” encompassing the solar atmosphere from the top layers of the convection zone up into the corona. The formation of jets such as dynamic fibrils, mottles, and spicules in the solar chromosphere are in the focus of such simulations.

Hansteen, Carlsson & Gudiksen (2007)

Courtesy, M. Carlsson
Simulations at large scales and high resolution (cont.)

Observed (top row) and synthetic (bottom row) Ca II 854.2 nm images at different positions in the line. **Left:** at $\Delta \lambda = -0.87$ Å; **middle:** close to the line core; **right:** in the line core at $\Delta \lambda = 0$ Å.
References


Boundary conditions for the magnetic field for run v10 and h20

**v10**

\[ B_{x,y} = 0 ; \quad \frac{\partial B_z}{\partial z} = 0 \]

**h20**

\[ \frac{\partial B_{x,y,z}}{\partial z} = 0 \]

outflow: \( \frac{\partial B_{x,y,z}}{\partial z} = 0 \)

inflow: \( B_y = B_z = 0, B_x = \text{const.} \)

\[ B_x = 20 \, \text{G} \]

→ back to § 17.
Growth of magnetic energy in the computational box of run h20 and mean absolute vertical magnetic field strength at a fixed geometrical height corresponding to the mean optical depth unity, $\langle \left| B_z \right| \rangle (\langle \tau_{500 \text{ nm}} \rangle = 1)$.

→ back to §17.