Reproducibility in Computational and Experimental Mathematics

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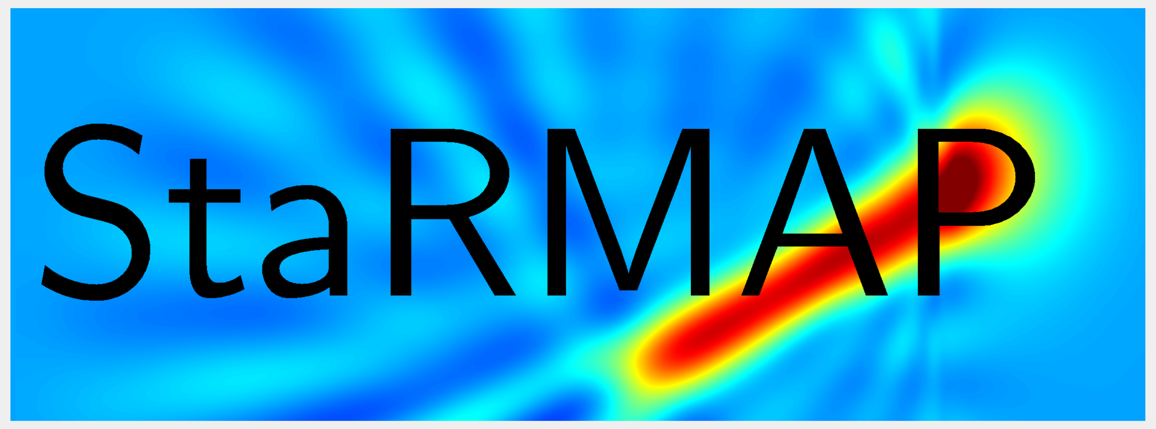

A Second Order Staggered Grid Method for Spherical Harmonics Moment Equations of Radiative Transfer

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Abstract

We present a simple method to solve spherical harmonics moment systems, such as the the time-dependent P_N and SP_N equations, of radiative transfer. The method, which works for arbitrary moment order N, makes use of the specific coupling between the moments in the P_N equations. This coupling naturally induces staggered grids in space and time, which in turn give rise to a canonical, second-order accurate finite difference scheme. While the scheme does not possess TVD or realizability limiters, its simplicity allows for a very efficient implementation in MATLAB. We present several test cases, some of which demonstrate that the code solves problems with ten million degrees of freedom in space, angle, and time within a few seconds. The code for the numerical scheme, called **StaRMAP** (**Sta**ggered grid **R**adiation **M**oment **Ap**proximation), along with files for all presented test cases, can be downloaded so that all results can be reproduced by the reader.

Radiative Transfer Equation for Photons in Medium

$$\partial_t\psi(t,x,\Omega)+\Omega\cdot\nabla_x\psi(t,x,\Omega)+\Sigma_t(t,x)\psi(t,x,\Omega) = \int_{S^2}\Sigma_s(t,x,\Omega\cdot\Omega')\psi(t,x,\Omega')\,d\Omega'+q(t,x,\Omega) \qquad (1)$$

Photon density ψ; absorption cross section Σ_a; scattering kernel Σ_s; total cross section $\Sigma_t=\Sigma_{s0}+\Sigma_a$; source q.

Spherical Harmonic Moment Methods

The P_N method (cf. [1]) conducts a Fourier expansion (spectral discretization) in the angular variable Ω; reduces high dimensionality; yields system of macroscopic PDE.

Efficient numerics recent subject of interest [5, 2, 1].

- Advantages over more direct discretizations: rotational invariance, no ray effect (cf. [3]).
- Drawback: Gibbs phenomena, i.e., spurious oscillations

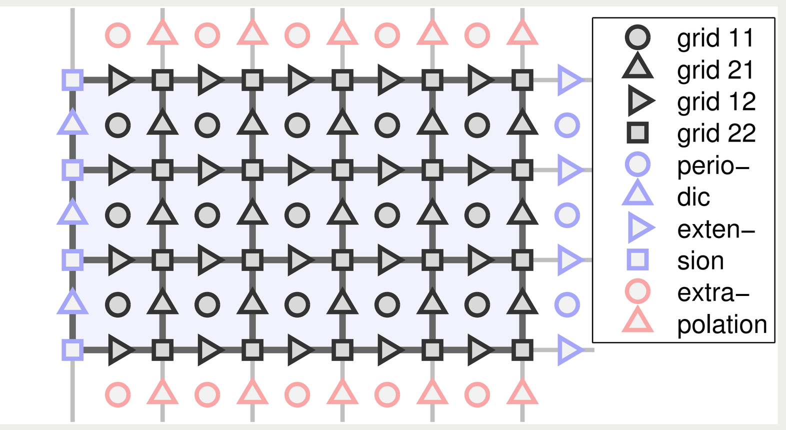
Also considered: Simplified P_N equations (SP_N) [4].

Gap: No P_N solver for general N available.

Moment system is hyperbolic balance law

$$\partial_t\vec{u}+M_x\cdot\partial_x\vec{u}+M_y\cdot\partial_y\vec{u}+C\cdot\vec{u}=\vec{q}\,, \qquad (2)$$

where the matrices M_x, M_y, C possess very specific patterns of their nonzero entries that admit the placement of the components of the solution vector $\vec{u}(x,y,t)$ on staggered grids.



Staggered grid of 5×3 cells; periodic b.c. in x; extrapolation b.c. in y; solution grid points (black boundaries), periodic extension points (blue), and extrapolation ghost points (red).

Features of This Project [6]

- Specific MATLAB files that encode P_N and SP_N matrices.
- Efficient solver file:
  - Place (based on matrices M_x and M_y) solution components automatically on appropriate staggered grids.
  - Store solution components as 2d arrays (= matrices). Compute FD stencils by shifting. Very fast in MATLAB.
  - Solver file employs special structure of parameters (e.g., isotropy, time-independence) to compute much faster.
- Examples files (few lines of MATLAB code) that call the other files. User hardly ever modifies non-example files.
- Solver file has defaults for every problem parameter and function, so an example file essentially is a prescription of how one deviates from the defaults.

Numerical Method

Central differencing in space:
$\partial_x w_{11}$ & $\partial_y w_{22}$ live on 21 grid; $\partial_x w_{22}$ & $\partial_y w_{11}$ live on 12 grid;
$\partial_x w_{21}$ & $\partial_y w_{12}$ live on 11 grid; $\partial_x w_{12}$ & $\partial_y w_{21}$ live on 22 grid.
Even components: on grids 11 and 22;
odd components: on grids 21 and 12.

Bootstrapping in time: Update even (odd) components from t to $t+\Delta t$, assuming that odd (even) components are constant. Thus system decouples into scalar ODEs

$$\partial_\tau u_k(x,y,\tau)+\bar{c}_k(x,y)u_k(x,y,\tau)=\bar{r}_k(x,y) \qquad (3)$$

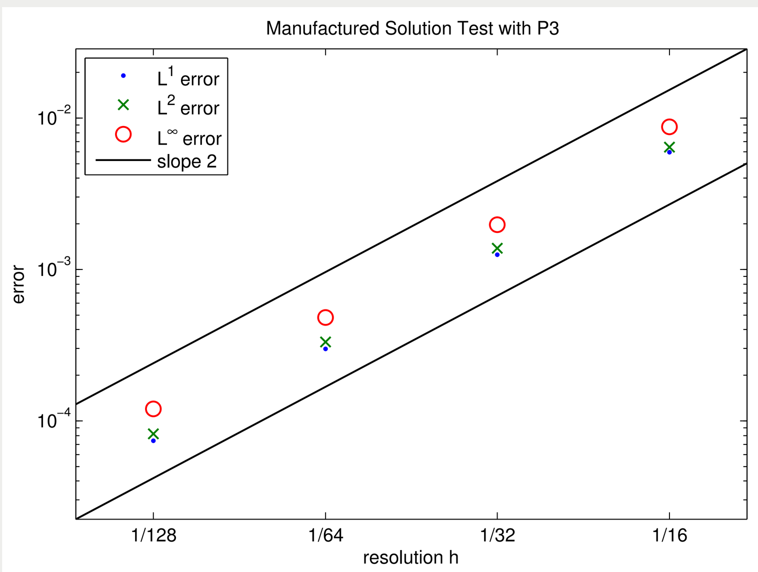
for $\tau\in[t,t+\Delta t]$. Evaluate $\bar{c}_k(x,y)=c_k(x,y,t+\frac{1}{2}\Delta t)$ and $\bar{r}_k(x,y)=r_k(x,y,t+\frac{1}{2}\Delta t)$. Exact solution of (3) is

$$u_k(x,y,t+\Delta t)=u_k(x,y,t)+\Delta t\,\big(\bar{r}_k(x,y)-\bar{c}_k(x,y)u_k(x,y,t)\big)\,E(-\bar{c}_k(x,y)\Delta t)\,,$$

where $E(c)=\frac{\exp(c)-1}{c}$.

Accuracy: 2nd order due to local symmetries.
Stability: Proof in [6].

Verification via Method of Manufactured Solutions (MMS)



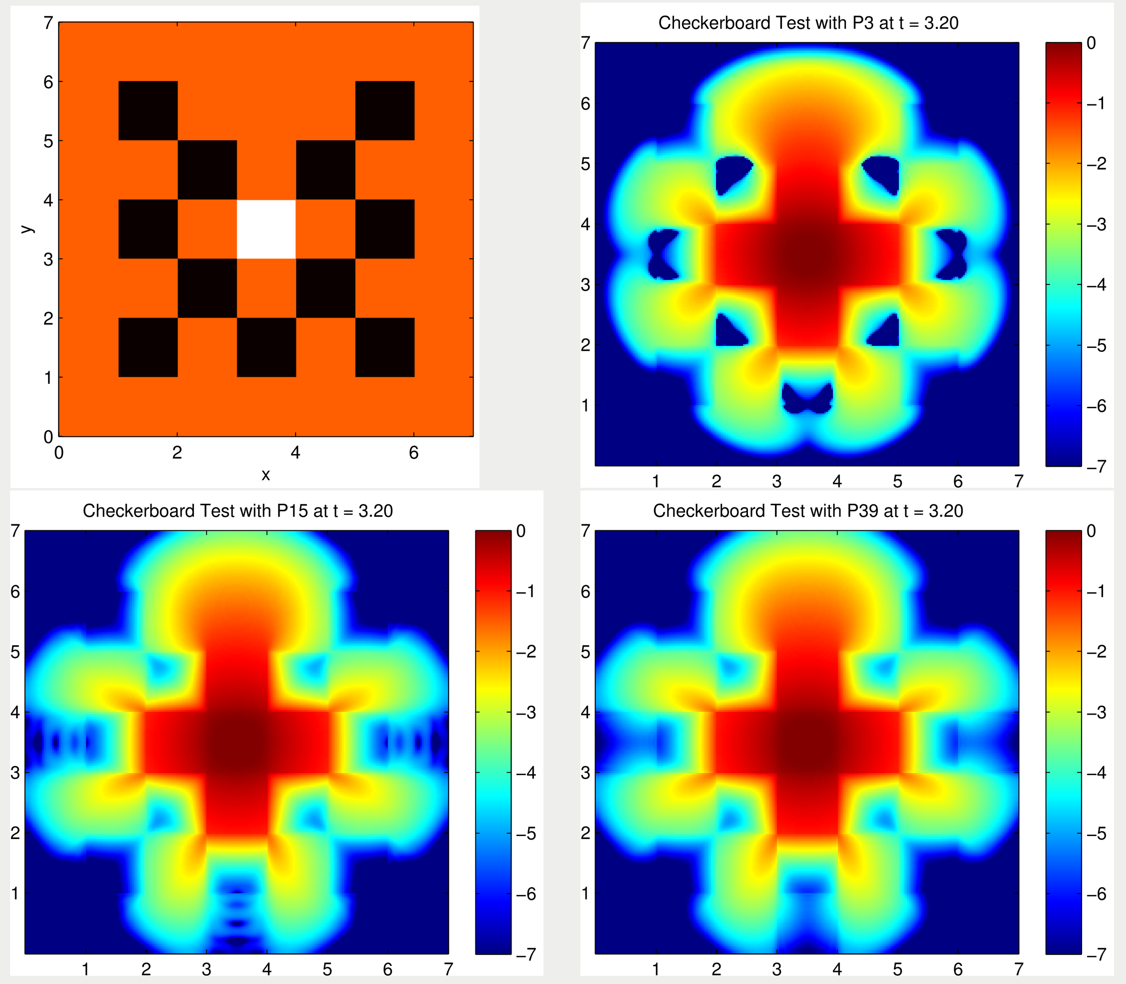
MMS: Choose a solution $\vec{u}(x,y,t)$. Then compute the source $\vec{q}(x,y,t)$ that generates this solution under (2).

Project Files Used by MMS Verification

Example file	`starmap_create_mms.m`
creates new file	`starmap_ex_mms_auto.m`
which calls P_N matrices constr.	`starmap_closure_pn.m`
and then solver file	`starmap_solver.m`

MMS source is computed via MATLAB's symbolic toolbox.

Checkerboard Geometry Test Case [1]



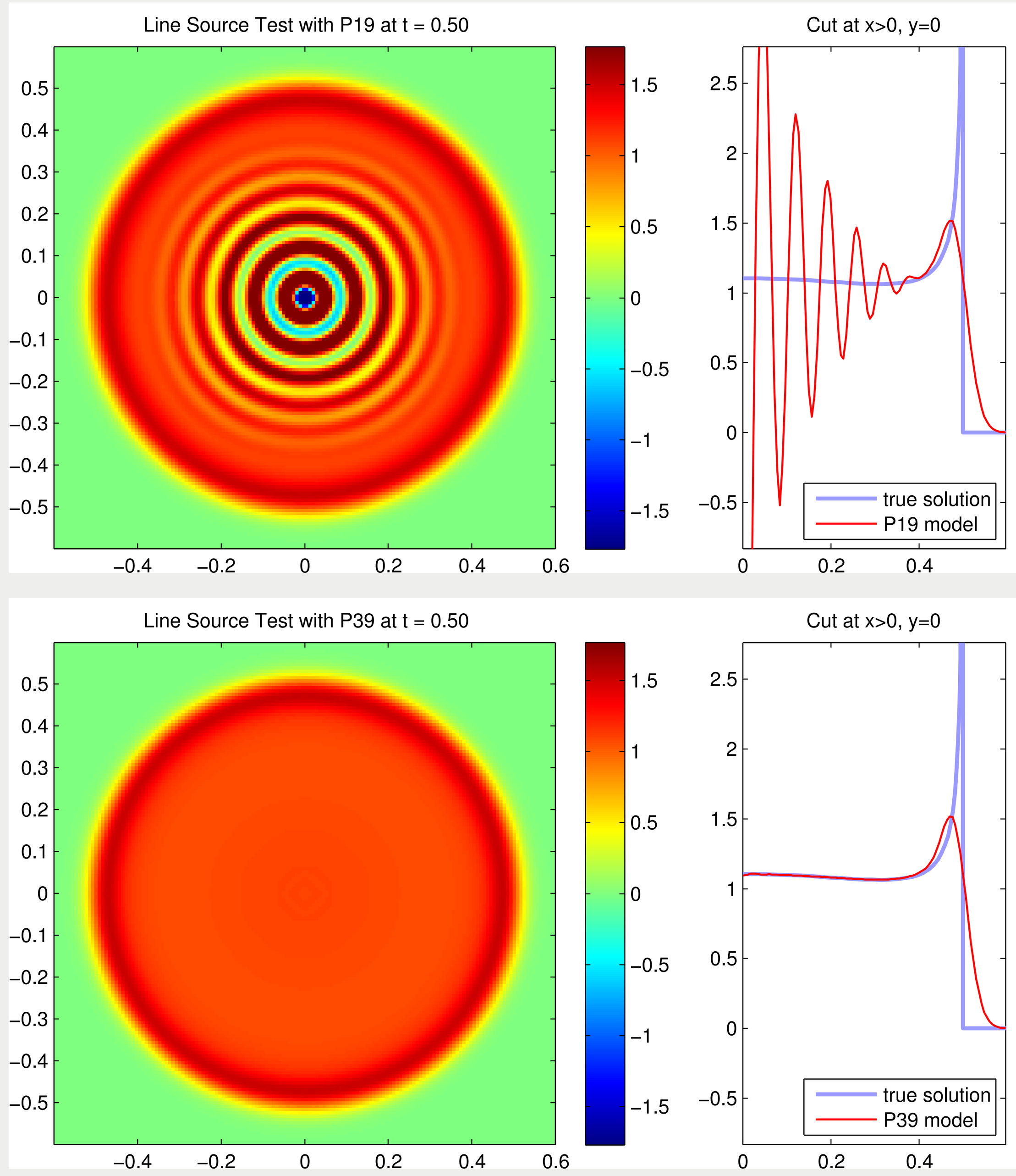
Project Files Used by Checkerboard Test Case

Example file	`starmap_ex_checkerboard.m`
calls P_N matrices construction	`starmap_closure_pn.m`
and then solver file	`starmap_solver.m`

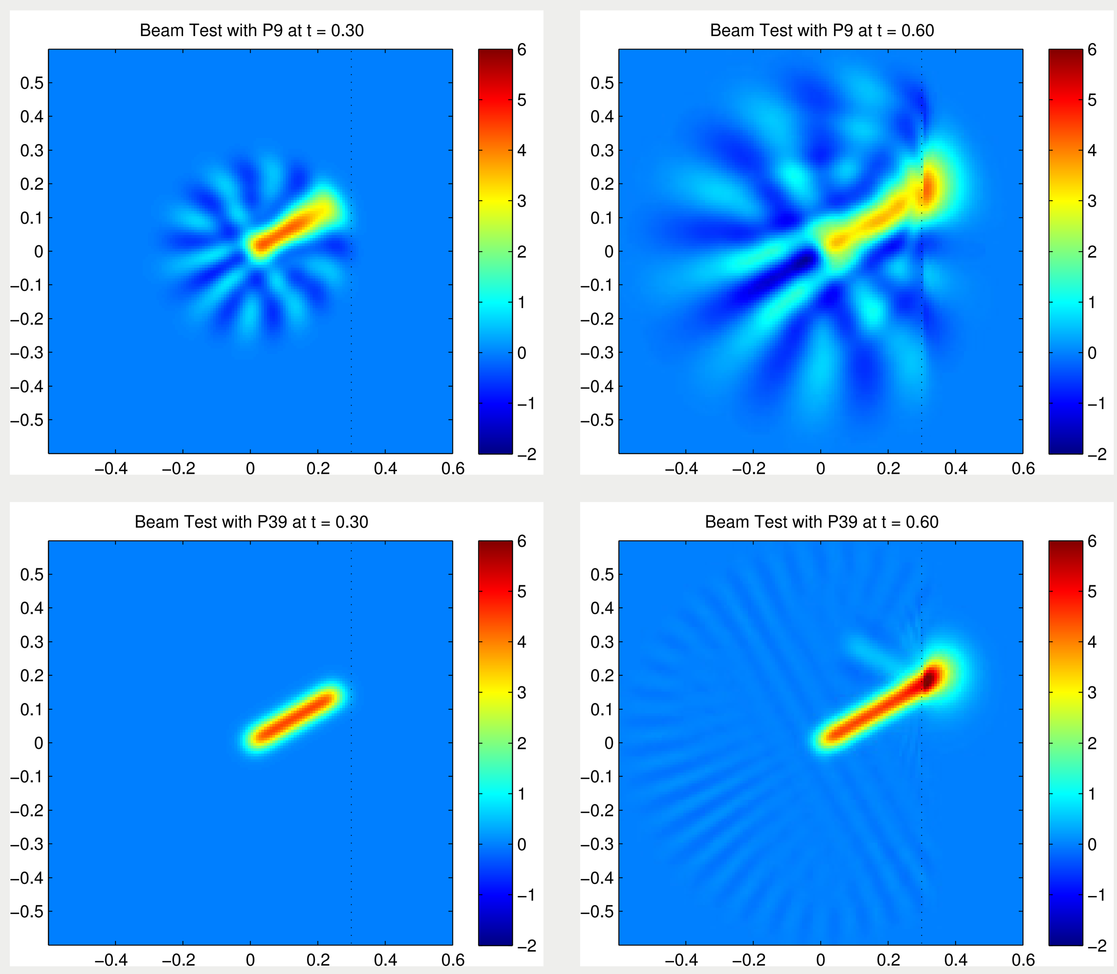
StaRMAP Example File for Checkerboard Test Case

```
function starmap_ex_checkerboard
%=========================================================================
% Problem Parameters
%=========================================================================
par = struct(...
'name','Checkerboard Test',... % name of example
'closure','P',... % type of closure (can be 'P' or 'SP')
'n_mom',5,... % order of moment approximation
'sigma_a',@sigma_a,... % absorption coefficient (defined below)
'sigma_s0',@sigma_s0,... % isotropic scattering coefficient (def. below)
'source',@source,... % source term (defined below)
'ax',[0 7 0 7],... % coordinates of computational domain
'n',[250 250],... % numbers of grid cells in each coordinate direction
'bc',[1 1],... % type of boundary cond. (0 = periodic, 1 = extrapolation)
't_plot',linspace(0,3.2,51),... % output times
'output',@output... % problem-specific output routine (defined below)
);
%=========================================================================
% Moment System Setup and Solver Execution
%=========================================================================
switch par.closure % define closure matrix function
case 'P', closurefun = 'starmap_closure_pn';
case 'SP', closurefun = 'starmap_closure_spn';
end
[par.Mx,par.My] = feval(closurefun,par.n_mom); % compute moment matrices
starmap_solver(par)
%=========================================================================
% Problem Specific Functions
%=========================================================================
function f = sigma_a(x,y)
% Absorption coefficient.
cx = ceil(x); cy = ceil(y);
g = (ceil((cx+cy)/2)*2==(cx+cy)).*(1<cx&cx<7&1<cy&cy-2*abs(cx-4)<4);
f = (1-g)*0+g*10;

function f = sigma_s0(x,y)
% Isotropic scattering coefficient.
cx = ceil(x); cy = ceil(y);
g = (ceil((cx+cy)/2)*2==(cx+cy)).*(1<cx&cx<7&1<cy&cy-2*abs(cx-4)<4);
f = (1-g)*1+g*0;

function f = source(x,y)
% Radiation source (only for zeroth moment).
f = 3<x&x<4&3<y&y<4;

function output(par,x,y,U,step)
% Plotting routine that uses logarithmic color scale.
V = log10(max(U,1e-20));
clf, imagesc(x,y,V'), axis xy equal tight, caxis([-7 0])
title(sprintf('%s with %s%d at t = %0.2f',par.name,par.closure,...
par.n_mom,par.t_plot(step)))
colormap jet(255); colorbar, drawnow
```

Line Source Test Case



Beam in Void and Medium



References

[1] T. A. Brunner and J. P. Holloway, *Two-dimensional time dependent Riemann solvers for neutron transport*, J. Comput. Phys. **210** (2005), no. 1, 386–399.

[2] R. G. McClarren, J. P. Holloway, and T. A. Brunner, *On solutions to the P_n equations for thermal radiative transfer*, J. Comput. Phys. **227** (2008), no. 3, 2864–2885.

[3] J. E. Morel, T. A. Wareing, R. B. Lowrie, and D. K. Parsons, *Analysis of ray-effect mitigation techniques*, Nucl. Sci. Eng. **144** (2003), 1–22.

[4] E. Olbrant, E. W. Larsen, M. Frank, and B. Seibold, *Asymptotic derivation and numerical investigation of time-dependent simplified P_N equations*, J. Comput. Phys. **to appear** (2012).

[5] G. L. Olson, *Second-order time evolution of P_N equations for radiation transport*, J. Comput. Phys. **228** (2009), no. 8, 3072–3083.

[6] B. Seibold and M. Frank, *StaRMAP — A second order staggered grid method for spherical harmonics moment equations of radiative transfer*, submitted to TOMS (2012).

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