Code Verification of MFIX Baseline Governing Equations

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  - Order of Accuracy Test
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- 2D Exact Solution
  - Rectangular Channel Case
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  - Governing Equations
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- Summary

Verification and Validation

- A framework for analysts and researchers to quantify the credibility of their computational simulations
- Verification addresses the correctness of the computer code and accuracy of the numerical solution to a selected model
- Validation assesses the accuracy and capability of the mathematical model in simulating the physics of interest
- Code verification assures whether the algorithm has been accurately in the software implemented and the numerical algorithm is consistent/ convergent and error-free
- Solution verification estimates numerical errors in solution: discretization, iterative, and round-off error

Order of Accuracy (OOA) Test

- Order of accuracy test: whether *observed order of accuracy* of the numerical computations matches the *formal order of accuracy* in the *asymptotic range*

- Formal order of accuracy is usually determined by the term with the lowest order in the truncation error expression

- Observed order of accuracy is the order at which the discretization error of the numerical solution reduces over a set of *systematically refined grids*

- Asymptotic range is defined as that range of mesh sizes (Δx, Δy, Δt etc.) where the lowest-order terms dominate the rest of the terms in the truncation/discretization error

Method of Manufactured Solutions (MMS)
(Roache and Steinberg, 1984)

- The concept behind MMS is that code verification deals with mathematics and thus doesn't require a physically meaningful solution

- A manufactured solution (MS) is an assumed solution based on which a modified set of governing equations and BCs are found for code verification

- Selection of manufactured solutions:
  - Smooth, analytical functions with smooth derivatives
  - Non-zero derivatives (including the cross-derivatives, if present)
  - Relative magnitude of terms should be of the same order
  - Realizable solutions (e.g., no negative temperature, density)

- Advantages and disadvantages

Method of Manufactured Solutions (MMS)

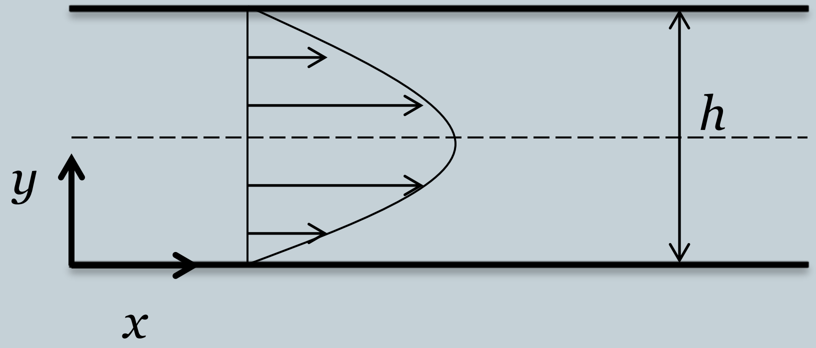
- Steps in performing order of accuracy test using MMS
  - Select appropriate manufactured solution (MS)
  - Obtain analytical source terms
  - Obtain the modified governing equations (original + source terms)
  - Solve the modified governing equations on multiple meshes
  - Obtain global DE norms for different mesh levels
  - Perform the order of accuracy test

- For evaluation of global DE norms, different norm definitions (L_1, L_2, L_∞) can be used

- If the observed order does not match the formal order, local discretization error can be studied in order to help isolate coding or implementation mistakes

2D Rectangular Channel Case

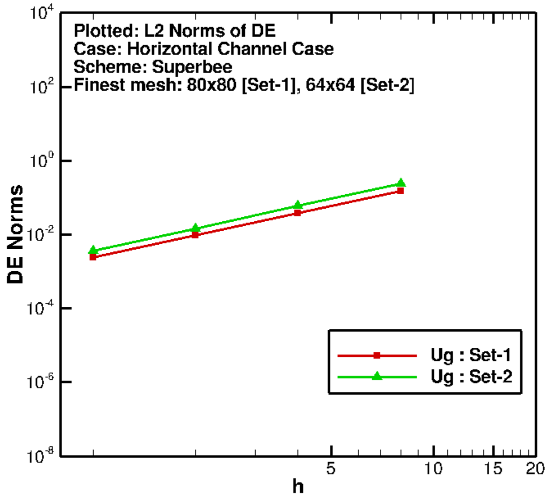
- 2D, Laminar, Navier-Stokes equations (Poiseulle flow)
- 2^{nd} order linear ODE, directly solvable for $dp/dx = \text{constant}$
- Single gas species, Cyclic (periodic) BC along x-direction, 2^{nd} order discretization scheme (Superbee)
- OOA tests on multiple mesh levels, for horizontal (x-momentum equations) and vertical (y-momentum equations) channels

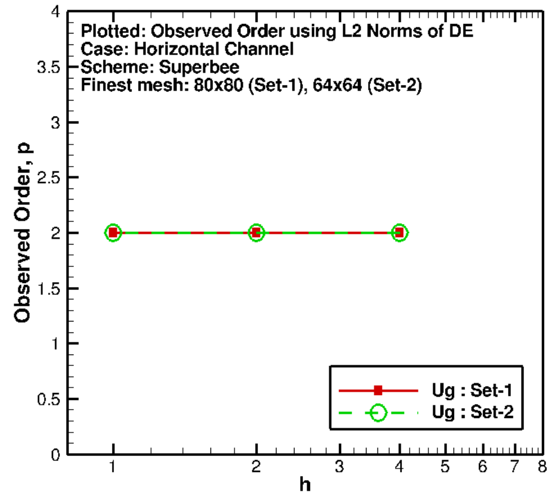


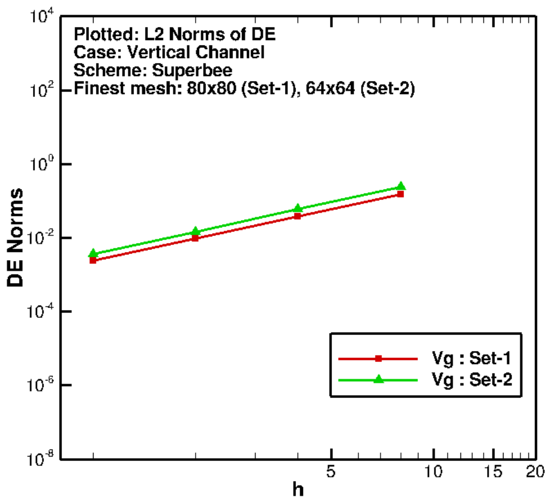
Gov. Equation: $\nu \dfrac{d^2u}{dy^2} = \dfrac{1}{\rho}\dfrac{dp}{dx}$

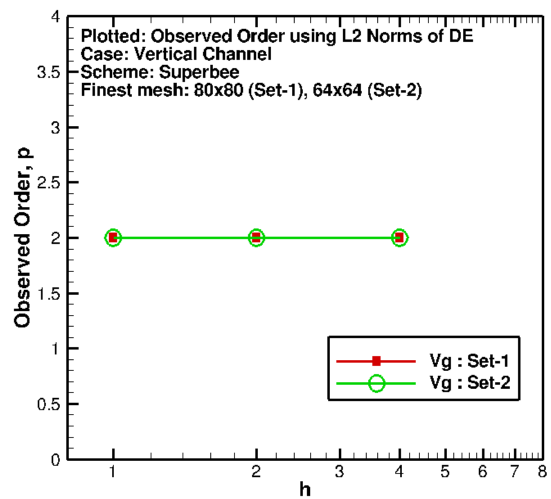
Solution: $u(y) = -\dfrac{dp}{dx}\dfrac{1}{2\rho\nu}y(h-y)$

2D Rectangular Channel Case









- Comments
  - 2nd order accuracy for these cases
  - Activation of limiters during transient phase
  - Better iterative convergence on 3D (i.e. with a few cells in z-direction) than 2D meshes
  - Linear initialization of pressure

Simplified MFIX Governing Equations

- Simplifications for MMS verification: Fluid-phase, single species, 2D, inviscid, incompressible

$$\textbf{Gas Continuity}: \nabla \cdot \left(\vec{v}_g \right) = 0$$

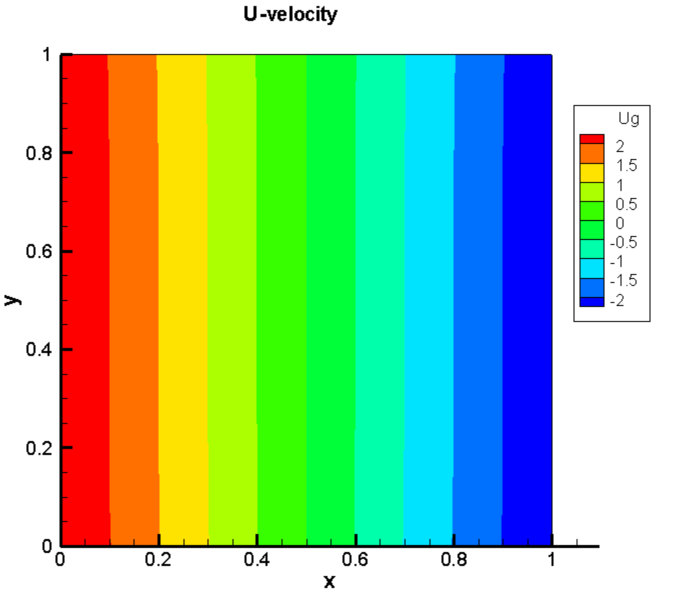
$$\textbf{Gas Momentum Balance}: \nabla \cdot \left(\vec{v}_g \vec{v}_g \right) = -\nabla P_g$$

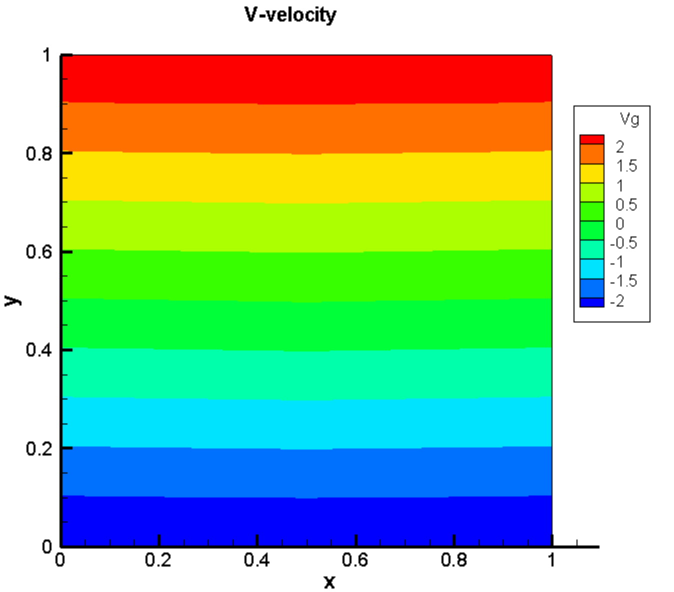
- Compressible solvers: Decoupled manufactured solutions

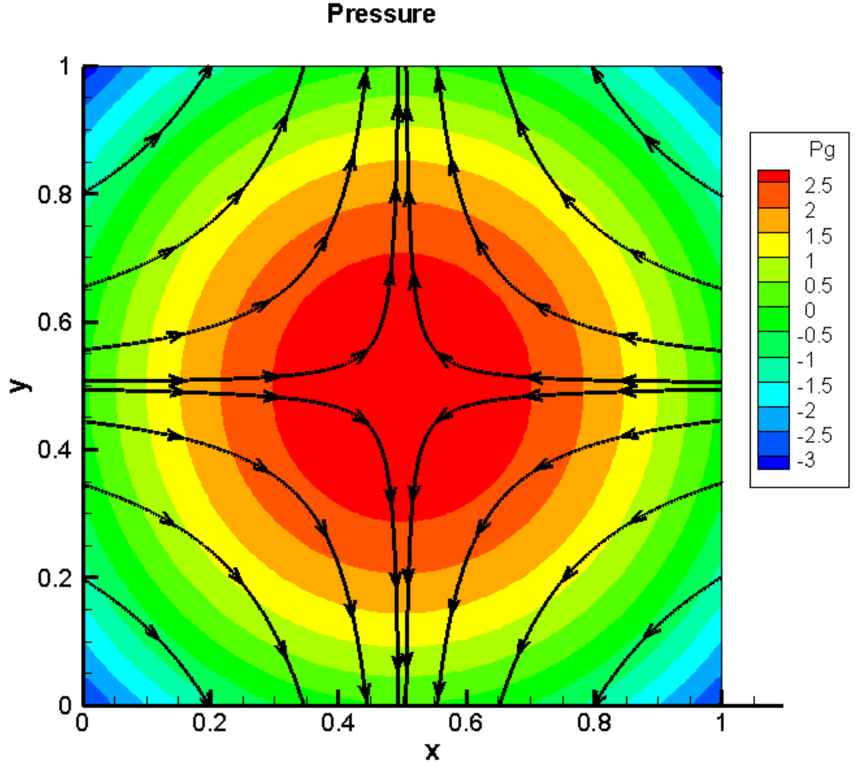
- Incompressible solvers: Velocity field must conform with the divergence free condition and the pressure field. For 2D:
  - Select u and v such that divergence-free condition is satisfied
  - Integrate momentum equations to derive pressure field

Eliminates the need for MMS source terms for these cases.

Polynomial Manufactured Solution



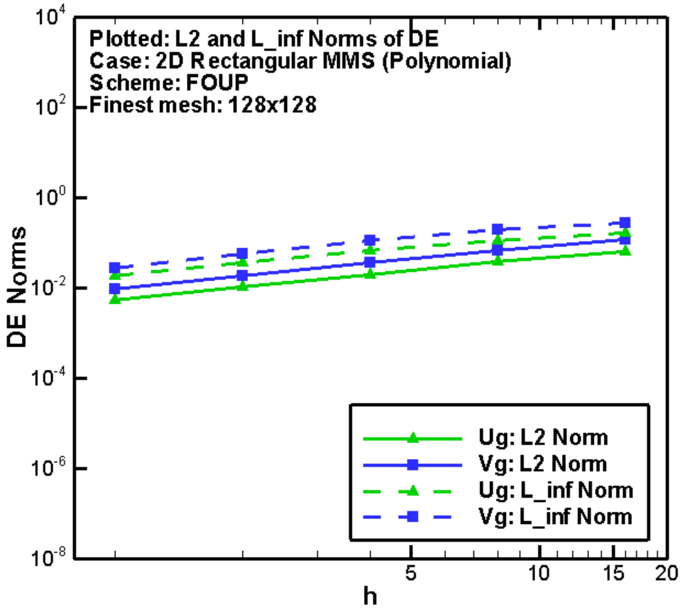


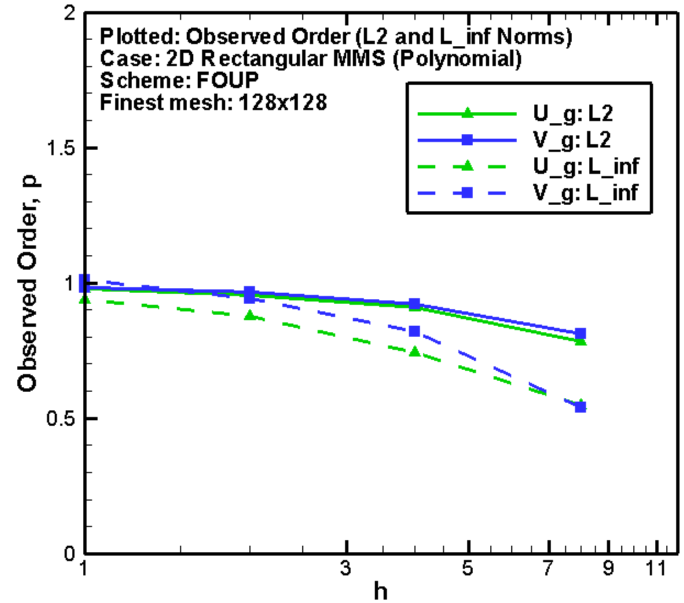


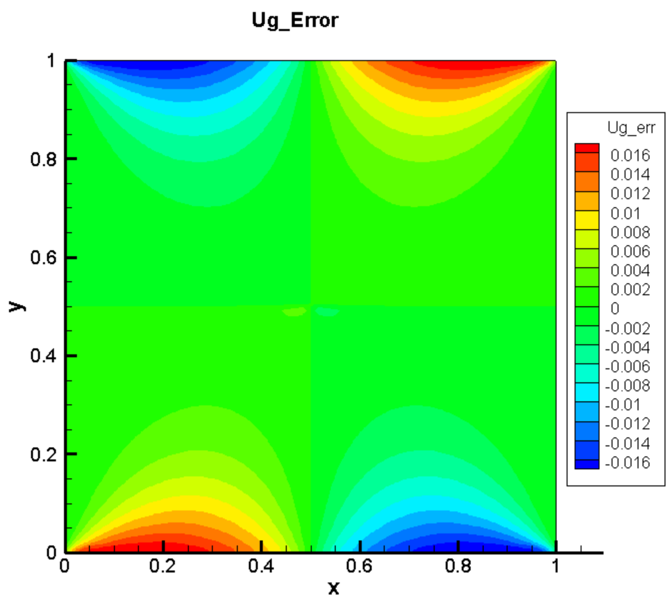
$$U_{MMS}(x,y) = u_0(0.5 - x)$$

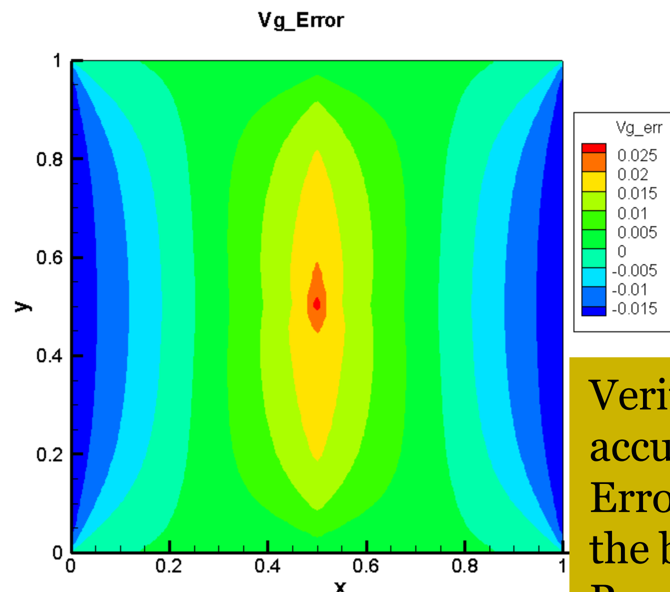
$$V_{MMS}(x,y) = -u_0(0.5 - y)$$

$$P_{MMS}(x,y) = P_0 + \frac{u_0^2}{2}(x^2 + y^2) - \frac{u_0^2}{2}(x + y)$$



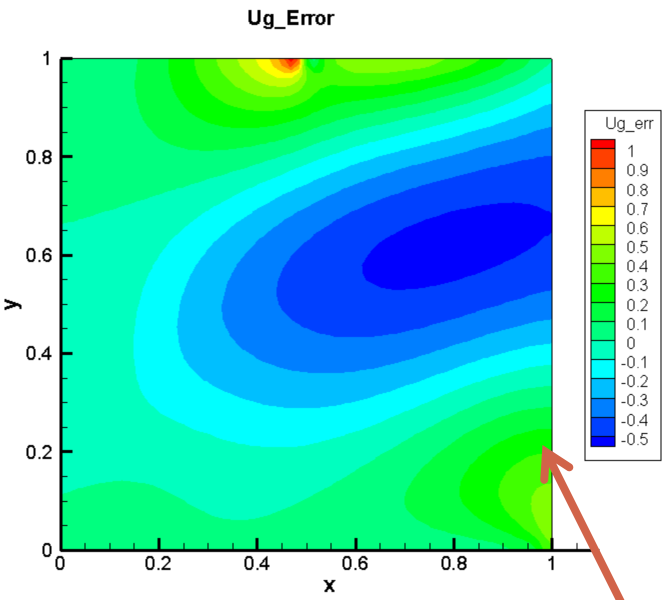


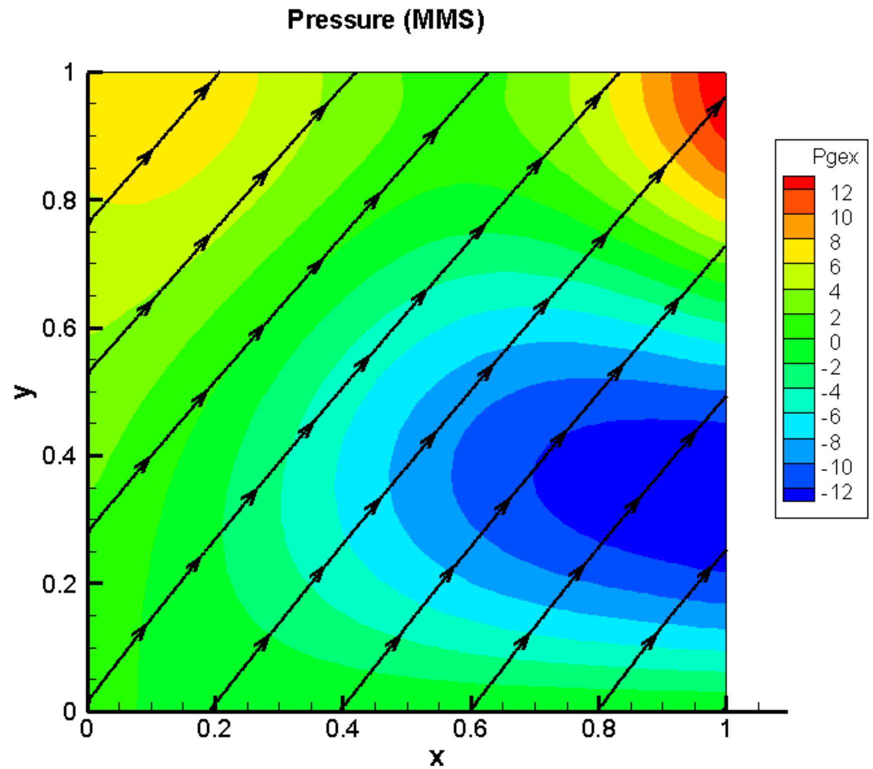


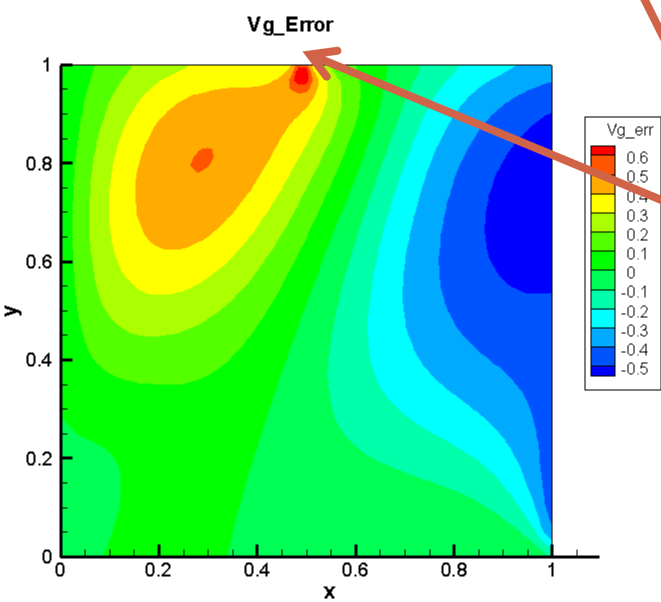


Verified 1st order accurate inside domain. Error accumulation at the boundaries. Possible issues with MMS BC specification.

General Manufactured Solution







- Errors at right and top boundaries possibly due to improper specification of BCs
- Need Dirichlet BC specification of all quantities at the boundaries

Summary and Future Work

- For the x- and y- momentum equations examined, the observed order matches the formal order for the code
- Separate MMS boundary condition specification option needed to apply Dirichlet values for different variables
- “Hooks” in the source code to apply MMS boundary condition and evaluation of MMS source terms -> (1) Single MMS input file from the user, (2) possibly an automated MMS verification-suite
- These simple verification cases pave the way for conducting MMS-based order of accuracy tests for MFIX for
  - 2^{nd} order discretization schemes
  - 2D and 3D meshes with variable mesh spacing
  - Governing equations in cylindrical coordinates
  - Multi-species, multiphase, unsteady governing equations
  - Various sub-models
  - Implementation of various BCs

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