

## Multi-Phase, Multi-Scale Mathematical Models of Splash Erosion

### Research History

After completion of an honours degree in applied mathematics at Monash University in Melbourne, Australia I was first introduced to the application of mathematical models and methods as a vacation scholar at BHP's Research Laboratories (now BHP-Billiton) in Melbourne, Australia applying analytical methods of electromagnetic theory for non-contact temperature measurement in the steel industry. Since then I have continued to apply mathematical methods to the solution of complex engineering problems within both academia and industry. This includes work as a research consultant in the Mechanical Engineering Department of the University of Wollongong involving the water-jet cooling of hot steel sheets and as a research scientist at Bluescope Steel Research Laboratories in Port Kembla, Australia improving commercial software used in the mathematical modelling of heat transfer and fluid flow within blast furnaces. As an Associate Research Fellow in the School of Mathematics and Applied Statistics at the University of Wollongong I applied analytical mathematical models to the pharmaceutical problem of drug delivery within swelling hydrogels. This resulted in the publication of eight papers in international conference proceedings including the Asia Pacific Microwave Conference, Computational Heat Transfer Conference, as well as the *ANZIAM Journal* and the *Computational Fluid Dynamics Journal*.

My PhD thesis work on the industrial problem of the "Mathematical Modelling of Water Drop Impact on Hot Galvanised Steel Surfaces" became the starting point for the construction, evaluation and solution of mathematical models of multiphase flow problems in engineering involving the complex interaction of multiple fluid phases and physical forces over a large range of length and time scales. This work resulted in the publication of three papers within the internationally recognised journal *Computers & Fluids*, *Computer Modelling in Engineering & Sciences* and *Engineering Applications of Computational Fluid Mechanics* as well as a workshop on Splash and Free Surface Flows. The most significant results of the PhD/postdoc work which are directly relevant to the fellowship application include:

- 1 Lagrangian Interface Tracking: I developed a second order accurate Lagrangian interface tracking algorithm (ITA) for multiphase flows which possesses several advantages over other interface tracking methods including the avoidance of instabilities of pure particle methods, a constant interface transition width, and an avoidance of the artificial numerical diffusion of fluid interfaces as well as artificial numerical surface tension.
- 2 Eulerian Multiphase Flow: The ITA was combined with a Godunov approximate projection method to ensure incompressibility up to second order while avoiding grid decoupling in the pressure and velocity without inducing instabilities for large, rapid changes of material properties across fluid interfaces so that artificial numerical boundary layers are not present within the flow.

My current research as a Research Associate in the School of Mathematics at Cardiff University is the further development of multiphase flow models of droplet dynamics in engineering and industry including computational studies of droplet break-up in uniform flow, multi-droplet interaction in spray impingement and the role of neighbouring droplets in the spray break-up process. The results of this research have recently been published in the proceedings of the European Conference on Liquid Atomization and Sprays as well as the *International Journal for Numerical Methods in Fluids*.

These results are a first stage in the development of highly accurate multi-physics, multi-phase, multi-scale flow models. Other than engineering and industrial applications the further development of such methods may be implemented in a wider context of the natural sciences including biological and hydrological flows.

I also have track record of popular presentations of science including invited public lectures on solar system formation and the mathematics of Leonardo da Vinci. I mean to continue to give other presentations as a way of furthering the understanding of science for the general public.

## Proposed Research

### A Background

“Nature favors those organisms which leave the environment in better shape for their progeny to survive” (James Lovelock, 1986)

There is no doubt that James Lovelock was referring to humanity in particular when he made this statement. As such, it has become more and more obvious that human survival depends closely on the health of the environment and issues such as human induced climate change are now a major global concern. Bad agricultural practices, overgrazing and deforestation are three contributing to factors which are exacerbated through soil erosion caused by water or wind. Soil erosion, especially water erosion, is one of the most important contributors to environmental and agricultural degradation. It is the main aim of this research proposal to elucidate the initial stages of the rainfall induced erosion process, the rainsplash phenomenon, which forms the basis of all empirical and predictive models of soil erosion and whose fundamental aspects are not fully understood.

It is estimated that worldwide 75 billion tonnes of the world’s agricultural soils are affected by erosion [1]. As a result there are both economic and environmental consequences [1, 2]:

- cropland becomes less productive because the soil left after erosion has lost its fertility and is unable to supply plants with the necessary nutrients
- the soil’s ability to retain water is decreased leading to an increased use of artificial fertilisers and a consequent pollution of rivers, streams, and lakes by agricultural nitrates and pesticides
- the eroded soil causes sedimentation in waterways which threatens aquatic life and hinders water flow
- the loss of seeds, seedlings, fertiliser and pesticides as well as the soil being washed from plant roots making them vulnerable to wind erosion
- extra cultivation needed to level out eroded surfaces and an increase of field operations as well as more fuel consumption and man hours

While soil erosion is a natural process human activities can substantially increase soil erosion beyond the natural rate becoming a process of degradation and so an identifiable threat to soil [4]. Typically, agricultural practices such as ploughing slopes, removing vegetative soil cover, overstocking, poor crop management and rotation as well as compaction by heavy machinery can expose land to the impact of rain or wind [4]. Soil erosion may become so severe that the land can no longer be cultivated and has to be abandoned. It is an important reminder that many agricultural civilisations declined due to land and resource mismanagement [5].

Water erosion is judged to be the more serious of the two types [2] and starts when a bare-sloped soil surface is exposed to rainfall, and the rainfall intensity exceeds the rate of soil water intake, the infiltration rate, or the soil is already saturated, leading to soil surface runoff [6]. It occurs in two stages: (i) detachment of soil particles by raindrop impact and splash (rainsplash or splash erosion), sometimes propelling soil particles into the air (saltation), or flowing water; and (ii) the transport of detached particles by splash or flowing water [4, 6].

Although water erosion starts at very small scales, involving raindrops and soil particles, its effects extend over larger scales when billions of raindrops fall on bare soil which can dislodge tons of soil per acre which is carried away by runoff [7]. These two-stage multi-scale processes are described in terms of [4, 8]:

- *Rainsplash Erosion*: soil particles are detached from the surface of the soil followed by transport of soil material away from the point of detachment
- *Sheet Erosion*: the removal of a thin uniform soil surface layer over a wide area by rainfall through unchannelled surface runoff
- *Rill Erosion*: an erosion process on sloping fields in which many randomly occurring small channels or rills with steep sides are formed by running water

- *Inter-rill Erosion*: erosion taking place in inter-rill areas
- *Ephemeral Erosion*: small channels eroded by concentrated flow forming in natural depressions
- *Gully Erosion*: water accumulates and often repeats in narrow channels or gullies which, over short periods, removes soil from a narrow area to larger depths
- *Bank Erosion*: wave motion in streams, rivers and lakes causing slumping of banks

### **A.1 Rainsplash Erosion**

The Process: It is clear that no erosion can occur unless soil detachment occurs first [9]. This makes the initial raindrop-impact-induced-erosion (RIIE) process of critical importance to agriculture. Despite its importance there is a lack of understanding of the fundamental processes involved in this phenomenon [6]. In fact, one of the central core actions of the First Soil Action Plan for England: 2004-2006, for the protection and better management of England's soils, is "Better Understanding and Information on Soils" due to the fact that 'there are still some large gaps in our scientific knowledge to fill...' [10].

Mathematical Models: While much experimental work has been done to understand the rainsplash process there is as yet insufficient field data, and the required monitoring networks do not yet exist, so that the assessment of erosion is only feasible by using mathematical models [3]. The recognition of the importance of raindrop splash in water erosion led to the development of erosion prediction models [11]. These models were developed in two main directions, firstly as purely empirical models such as the universal soil loss equation (USLE) to predict sheet, rill and inter-rill erosion and secondly the more process based models such as that of the Water Erosion Prediction Project (WEPP) and the European soil erosion model (EUROSEM). It must be stressed that while the second of these model types are an improvement on simple empirical or statistical models they make use of bulk properties developed from reasonable phenomenological assumptions and tend to express larger scale kinds of erosion such as rill and gully erosion. Apart from experimental studies little has been done to model the actual rainsplash process itself.

Multi-Scale: Raindrop impact induced erosion is a complex process related to the transport of solid granular particles via a fluid phase, either a liquid, or flowing granular phase spanning a large range of spatial and temporal scales. However, it is still very difficult to provide a consistent description of particle laden flows either from a one phase or two phase point of view [12]. A mathematical model of this process must be able to deal with an inherently multi-scale phenomenon:

*Spatial scales*: ranging from soil particulate dimensions, such as clay (0.002 mm), silt (0.002-0.05 m), sand (0.05-2 mm) and gravel (2-75 mm); to droplet sizes, including light rain (0.5-2 mm), moderate rain (1-2.6 mm) to heavy rain (1.2-5 mm) and secondary splash droplets <0.5 mm; soil crater diameters ~6 mm for a 3 mm drop at terminal velocity; diffusion path lengths in soils, pore sizes.

*Temporal scales*: for a 3 mm drop impacting at terminal velocity, time scales range from the compressibility time scale ~ 2  $\mu$ s, convective time scale ~0.4 ms, droplet spreading timescale ~1 ms, full splash with ejected secondary droplets ~7 ms.

Sub-processes & Stages: RIIE is a two stage process and results from raindrop impact and flowing water acting either singly or together resulting in the identification of four sub-processes, raindrop detachment (RD) with transport by: (a) raindrop splash transport (RD-ST), (b) raindrop-induced flow transport (RD-RIFT), (c) flow transport (RD-FT) and (d) flow detachment (FD) by flow transport (FD-FT) [9]. In RD-ST raindrop energy detaches soil particles and also expels the particles from the impact site. In RD-RIFT bulk water flows, from the impact of multiple droplets, are penetrated by other raindrops to further detach soil particles and lift them into the flow, so-called flow suspension (FS), or splash them and then

move the particles downstream. RD-FT, on the other hand transports soil particles directly with the flow without a need for raindrops and FD-FT occurs when the flow overcomes the cohesion and inter-particle frictional forces beyond a critical stream power [9]. In each case these phenomenological distinctions are a product of several factors influencing splash detachment: (i) raindrop erosivity - depending on drop size, shape and kinetic energy, (ii) target characteristics - depending on soil texture, moisture content, micro-topography and the presence of a water film and (iii) the behaviour of a water drop on impact with the soil surface [13]. The water drop impact process can be divided into three stages [11, 13, 14]:

- *Impact* - the collision and deformation of a falling raindrop at the surface
- *Splash* - the rupture and collapse of the drop into a thin disc of fluid splaying radially outwards and the ejection of daughter droplets from the point of impact
- *Cratering* - the process of cavity formation by the impacting drop as it penetrates the soil

Multi-Drop: There are also distinct differences between the impacts of a single drop to that of multiple droplets [13] although the terminology in the literature lacks clear definitions since many researchers isolate and examine singular aspects of splash such as single raindrop collision behaviour, raindrop erosivity or soil susceptibility to splash [13]. As such, rainsplash is in fact a complex geomorphological process involving the combination of various splash sub-processes or mechanisms each governed by the interaction of numerous parameters [13].

Conclusions: The rainsplash process, being the source of water erosion at larger scales, remains the least understood. Current mathematical models can capture some of the empirical and statistical aspects of the process or predict soil erosion using phenomenological assumptions of bulk properties but cannot describe the detailed structure of this multi-scale process. There is a need to understand the rainsplash process in greater detail and thereby justify or correct many underlying assumptions within current models. For this reason I mean to develop, validate and solve a mathematical model which directly models the fluid dynamical and particulate aspects of the rainsplash process.

## **B Project Outline**

### **B.1 Aims**

It is the central aim of this proposal to construct and numerically solve a multi-phase, multi-scale mathematical model for the rainsplash process. Environmental concerns have made the choice of such a project particularly timely as well as for the following reasons:

- 1 While previous research has been focused on the solution of multi-fluid flow problems, flow through stationary porous media and the problem of soil ploughing and tilling, to the author's knowledge, no model has yet been developed which can treat all three problems at once with a single uniform approach.
- 2 Much experimental work has considered the single drop-soil impact problem with very few studies for the interaction process of multiple drop impacts. Many models upscale empirical single-drop results to multi-drop impact, this approach remains to be justified [29].
- 3 The fundamental rainsplash process remains the least understood for which the solution of a mathematical model would provide essential information involving:
  - Soil surface detachment and saltation, particle flow transport and crater formation
  - Validation or correction of previous upscaled models such as USLE, WEPP and EUROSEM
  - A way to test the influence of individual forces affecting the process and so determine how these forces interact
  - A way to derive previously used assumptions for parameters of the erosion process such as: the weight of soil detached by a raindrop, soil detachability, the rate of rainfall detachment, sediment deposition rate and so on [9].

To satisfy these aims the model must be able to fulfil certain requirements and a choice must be made regarding the types of models already available or whether a new modelling approach needs be developed.

### **B.1.1 Model Requirements**

Physical Aspects: a mathematical model of the rainsplash process should be able to include various physical aspects of the phenomenon including: the ability to model three separate phases, two fluid and one solid phase. In some cases the size of the granular phase can be representative of the length scale of the problem e.g. when the fluid phase carries in it a suspension of soil particles which are not necessarily negligible in size. That is, the solid phase occupies a non-negligible volume, is of a given mass and maintains itself as a rigid body. As well, the fluid-solid phase boundary should be of the no-slip type and the particle can possess irregular as well as regular shapes. In some instances the solid particles may undergo material deformation requiring a constitutive law which may be expressed through, for example, an elastic solid. Other than linear translation the particles may also undergo rotation due to impacts with other particles or under certain flow conditions.

Model Construction: there are three aspects for simulating the rainsplash process, firstly to formulate the physical principles involved followed by a mathematical model based on those principles and thirdly to construct a computational model of the mathematical one. The computational model should possess several characteristics including: numerical accuracy, robustness, stability, fidelity and convergence.

### **B.1.2 Computational Model Types**

Currently, there are a range of ways to solve the system of partial differential equations, with their associated boundary and initial conditions, making up the mathematical models defining multiphase flow or granular materials. There are generally three such types: Eulerian, Lagrangian and hybrid Eulerian-Lagrangian (HEL). In purely Eulerian models all system variables are field variables defined on a grid. However, advective forces used to move solid granular particles are not as easily included. Lagrangian models on the other hand are well suited to model the motion of particles but not diffusive flow. Hybrid Eulerian-Lagrangian methods promise to treat both particulate and field variables in a consistent manner. It is the way in which the Eulerian and Lagrangian methods are used that differentiates the various model types.

In recent years purely Eulerian or Lagrangian methods have gone out of fashion based on the ability of hybrid methods to treat separate Eulerian or Lagrangian aspects more efficiently. Some of the more well known methods involving the modelling of fluid-structure interaction include:

Discrete Element Method (DEM): DEM [15] is a Lagrangian method which was originally designed to model the behaviour of granular materials as distinct particle elements so capturing the discontinuous property of the materials. Granular particle motion is modelled through mechanical interaction between two dimensional circular elements and the boundaries.

Immersed Boundary Method (IBM): the IBM is an HEL which was designed for the simulation of flows (the Eulerian component) with immersed elastic boundaries (the Lagrangian component) such as muscle contraction in the heart. It may also be used to model fluid-structure interaction through very stiff elastic bodies although this can lead to numerical instabilities [16]. Thereby the fluid-structure is tracked automatically without needing to update a Lagrangian mesh. Its main disadvantage is that immersed structures are one-dimensional carrying mass but no volume [16]. To circumvent these problems the *Immersed Finite Element Method (IFEM)* allows non-uniform grids which do not have to follow the

motion of the fluid-structure interfaces [17].

Particle-in-Cell Method (PIC): In the PIC method the Lagrangian particles are not assigned a physical dimension and do not undergo any particle-particle interactions, instead the particles are used to advect physical variables whose information is mapped to an underlying Eulerian grid where the momentum equation is solved. An improved version of the PIC method is the *Material Point Method (MPM)* which is also able to consider inter-particle grain interactions through a contact algorithm as was done in the IBM and can model inter-particle sliding or bonding, it avoids numerical diffusion and can model plastic strain [18].

Immersed/Global Phase Method (GPM): In the immersed phase method the approach first detailed in [19, 20] is used to model both fluid and solid aspects of the rainsplash process. This is an HEL method which can model the fluid and solid parts of the problem in a unified way by assuming that both solids and fluids may be approximated as fluids with a given density and viscosity. The soil particles are modelled as rigid solids with high viscosity so that the no-slip condition is automatically satisfied at the fluid-solid boundary. Field variables: velocity, pressure, density and viscosity are defined on a fixed Eulerian grid whereas the Lagrangian component of the method permanently traces the identity of phase being either one of the two fluid phases or the solid phase. This method is a generalised version of the GMPP scheme I developed to model multiphase flow [19, 20].

## B.2 Objectives

The aims and modelling aspects referred to in Section B.1 must be realised into a set of objectives for the proposed research to answer in a sequential manner:

1. The development, validation and application of a two-phase flow model able to accurately simulate moving boundary problems and capture deforming and disrupting fluid interfaces
2. The development, validation and application of a three-phase flow model which satisfies the requirements of objective 1 and can also include the transport of small suspended granular particles
3. The development, validation and application of a granular particle model able to accurately represent soil porosity, sedimentation, water transport and soil particle mobilisation
4. The development, validation and application of a unified three-phase, air-water-soil, model connecting and satisfying objectives 1, 2 and 3 and able to model the rainsplash phenomenon

## C Programme & Methodology

### Objective 1

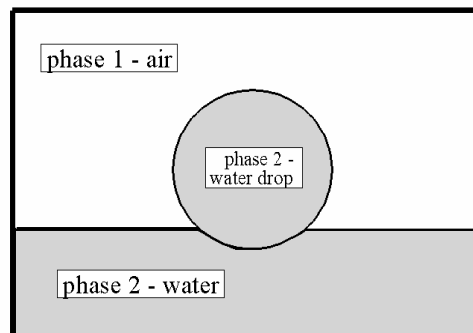


Fig 1: the two-phase drop splash process

*Overview:* The mathematical model must be able to provide detailed and accurate simulations of the droplet deformation and impact process, see Figure 1, whether at normal or oblique impact, on plane or rough surfaces, including the spreading and splashing phenomena as well as secondary droplet expulsion. This involves inertial, viscous, gravitational and surface tension forces as well as a moving contact line for drop-surface interactions [21].

*Methodology:* I will make use of my previously developed incompressible multiphase flow algorithm, the Godunov Marker Particle Projection Scheme (GMPPS), combining an accurate interface tracking algorithm using a Lagrangian particle method, the Marker-Particle (MP) method [19], and an Eulerian flow algorithm [20] which is a subset of the more general Global Phase Method discussed in Section B.1.2. This approach is a one-field (OF), hybrid Eulerian-Lagrangian (HEL) (mesh-particle) method where a single domain captures the entire flow including multiple fluid phases. The velocity and pressure are discretised on an underlying fixed Eulerian grid whereas fluid phase information or colour is advected through the grid as Lagrangian particles so that grid density and viscosity may be reconstructed from particle information. The method has been successfully applied to the droplet-solid impact problems [22] as well as the drop deformation and break-up problems [23]. It possesses several advantages over other methods including:

- a uniform approach to complex fluid dynamics problems involving multiple interacting fluid phases
- a method with an inherent multi-physics ability to incorporate inertial, pressure, viscous and surface tension forces
- a second order accurate approximate projection method which avoids spurious checkerboard modes
- Godunov discretisation of convective terms in the Navier-Stokes equations correctly matching velocities across fluid interfaces and avoiding cell Reynolds number restrictions
- an ability to track fluid colour at the sub-grid scale level without loss of information maintaining fluid phase identity permanently

The MP method will always advect fluid bodies faithfully, even if the body cannot be supported on the grid, and is very robust for flows with strong vertical content which are especially prevalent when fluid bodies undergo severe topological changes such as in the case of the rainsplash phenomenon [24].

## Objective 2

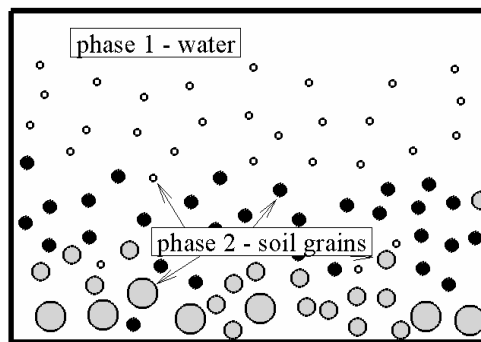


Fig 2: two-phase suspension flow

*Overview:* this is a three phase problem, two fluid and one solid, which can be treated in a number of ways. For example Figure 2 shows the case where the second fluid phase, air, is not involved and the solid phase is suspended purely within the water phase. One possibility is to treat the granular phase as a high viscosity fluid and so incorporate it into a one-field method such as proposed for objective 1. A second option is to treat the third phase as a solid which is moved with the fluid velocity and does not take into account mutual particle-particle

interactions.

**Methodology:** the incorporation of a third granular phase to represent soil particles in suspension is easily incorporated within GPM methods, including the two-phase GMPP scheme. One advantage of OF-HEL models is that they can incorporate the effects of ordinarily unresolvable scales, such as microscopic soil particles, within the resolvable scale through the sub-grid scale resolution available within the Lagrangian particle component. Soil particles are then advected with the flowing/granular phase velocity by solving a Lagrangian equation of motion.

### Objective 3

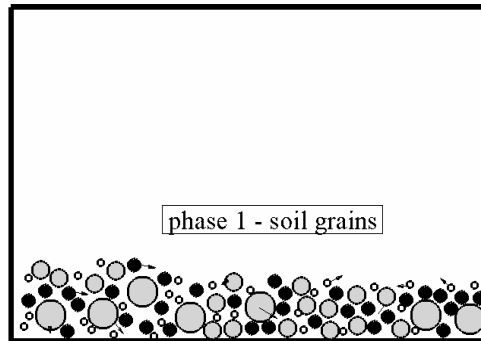


Fig 3: single-phase granular flow

**Overview:** the soil phase represents a collection of grains forming the soil matrix with interconnected pore spaces which are available as channels for water and solute transport and can lead to swelling and shrinking of the soil [25], see Figure 3. Any model must also be dynamic having the ability to model the processes of detachment and mobilisation of soil particles [22]. In addition it should be able to include particle-particle and particle-fluid interaction such as elastic impact or viscous damping (elastohydrodynamics), soil cohesion and friction for regular and irregularly shaped particles [26, 27].

**Methodology:** A method of purely soil particle interactions including arbitrary particle geometry, particle frictional and cohesive forces is already available through the discrete element method (DEM) and its extensions [15] and will be used to achieve this objective. This is a single-phase method representing the granular phase, grain movement and interaction.

### Objective 4

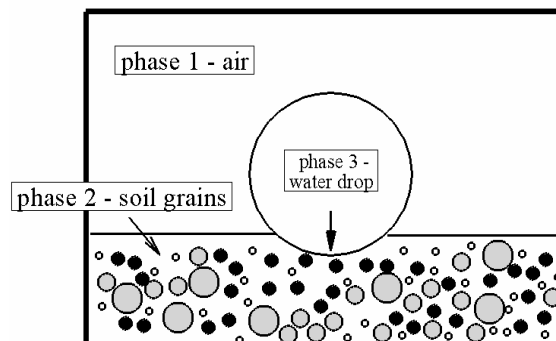


Fig 4: the full three-phase rainsplash process



Overview: this model must be able to incorporate the aspects displayed by the models of objectives 1-3 including: two-phase flow with surface tension, two-phase suspension flow, single-phase granular flow and three-phase, two-fluid suspension flow with general granular particles, see Figure 4. The model must include gravitational, viscous and surface tension forces as well.

Methodology: This is a more complex problem than any of the other three methods proposed in objectives 1-3. However, the approach remains the same. In this instance we require a multi-phase method to deal with the fluid dynamics of splashing such as the OF-HEL method of objective 1 in combination with a Lagrangian technique which is able to incorporate particle-particle force interaction and the particle-fluid force interaction. This can be achieved with a version of the GP method by incorporating the DEM method of objective 3.

## Timeline

Objectives 1-3 are designed to be carried out sequentially, first 1 followed by 2 and so on. Objective 1 lies directly within my own field of expertise and an OF-HEL code already exists. It will be used as a basis for the other computational models to be developed for objectives 2-4 by expanding it as a Global Phase Method proposed in Section B.1.2. The application of the GMPPS code to objective 1 is already at least partially complete. There remain some issues relating to more accurate and faster simulations which should be completed relatively quickly within the first year of the fellowship. The development of the method for the subsequent objectives, the construction and validation is expected to take the rest of the first year and part of the second. The applications for objective 2-4 are to be achieved by the second year. The extension of the GPM to the full rainsplash problem is expected to be straightforward and the remainder of the second year will be taken up with the validation and application of the full code.

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