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Research on Verification and Validation Strategy of LAD2D for Detonation Fluid Dynamics

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Contents

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- Introduction
- The Detonation Models
- LAD2D Code
- V&V Strategy of LAD2D
- Parts of Results of V&V
- Conclusion and Suggestions

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Introduction(1)

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- In the fields of science and engineering, a great many of problems are a complex process with multiphysical coupling.

Aeronautics

Medicine

Building

Accident occurrence

Nuclear engineering

Water Dynamics

Introduction(2)

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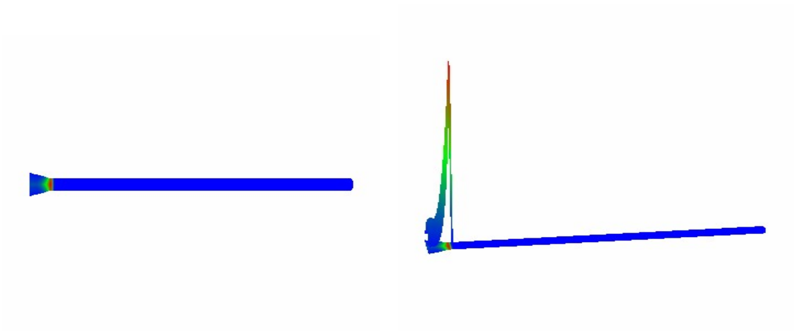
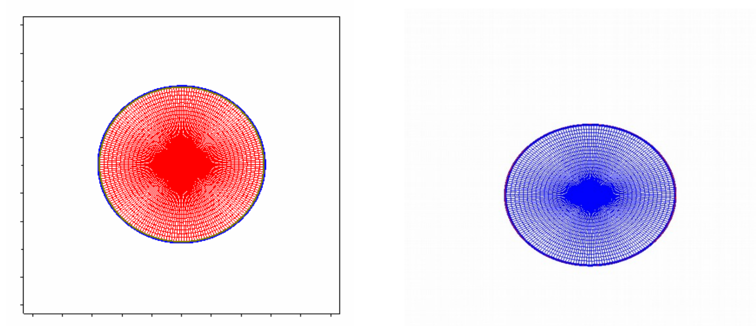
- These multiphysical processes are usually described by high nonlinear partial differential equations; it is difficult to find the analytical solution.
- During the last three or four decades, numerical simulations of multiphysical processes is playing increasingly important in scientific research or in the analysis and design of engineering.

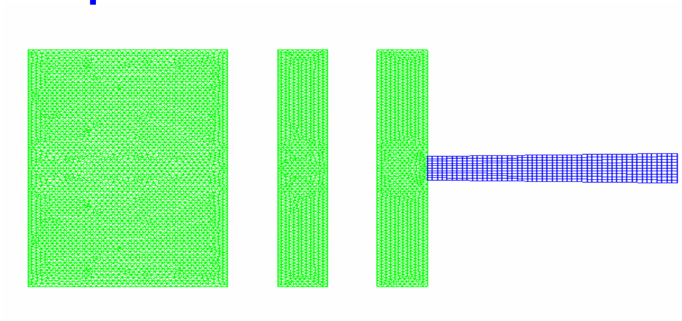
Detonations and Combustions



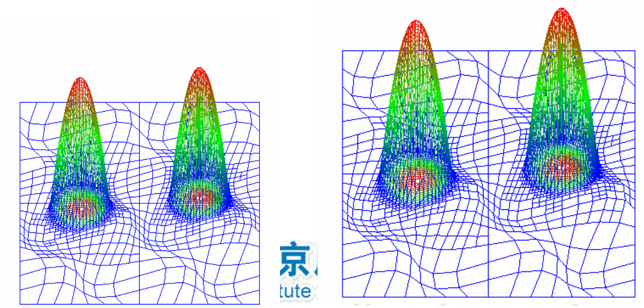
Implosion problems



Explosion and shock waves



initial and boundary value problems



Introduction(3)

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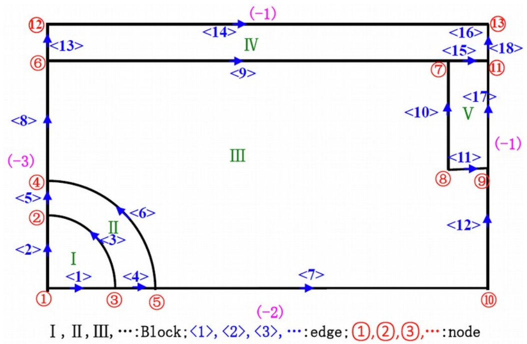
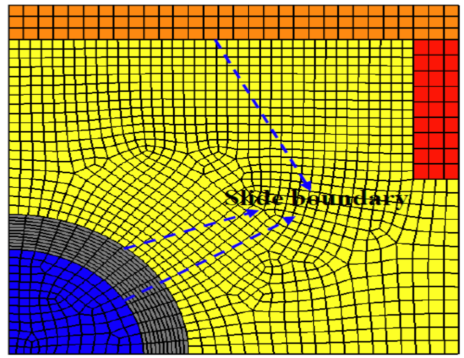
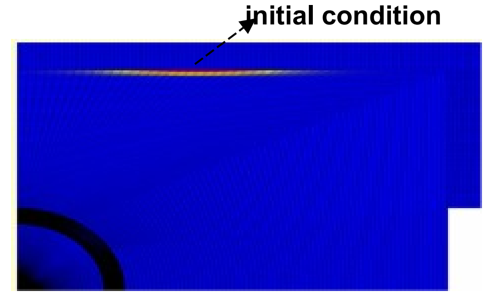
- Basic steps of computational simulation



1. Geometry and domain

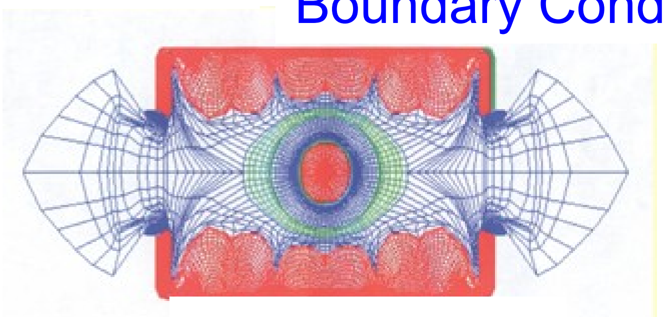


2. Generation mesh



3. Apply Loads and Boundary Conditions

4. Computational Analysis



5. Visualization

Errors and uncertainties in simulation code predictions have many sources, including the lack of knowledge of the underlying physics models, the variability of the initial geometry and materials, and degree of variability in the physical phenomenon itself. **Errors and uncertainties may generate in each simulation Process**

Introduction(4)

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- With the increasing reliance on simulation codes, it is becoming critically important to determine how well they predict actual physical phenomenon.
- Users and developers of computational simulations codes today face a critical issue: How should confidence in modeling and simulation be critically assessed?
- The verification, validation and uncertainty quantification (V&V&UQ) of computational simulations are the primary methods for building and quantifying this confidence. Goal is to estimate and minimize uncertainty in predictions.

Introduction(5)

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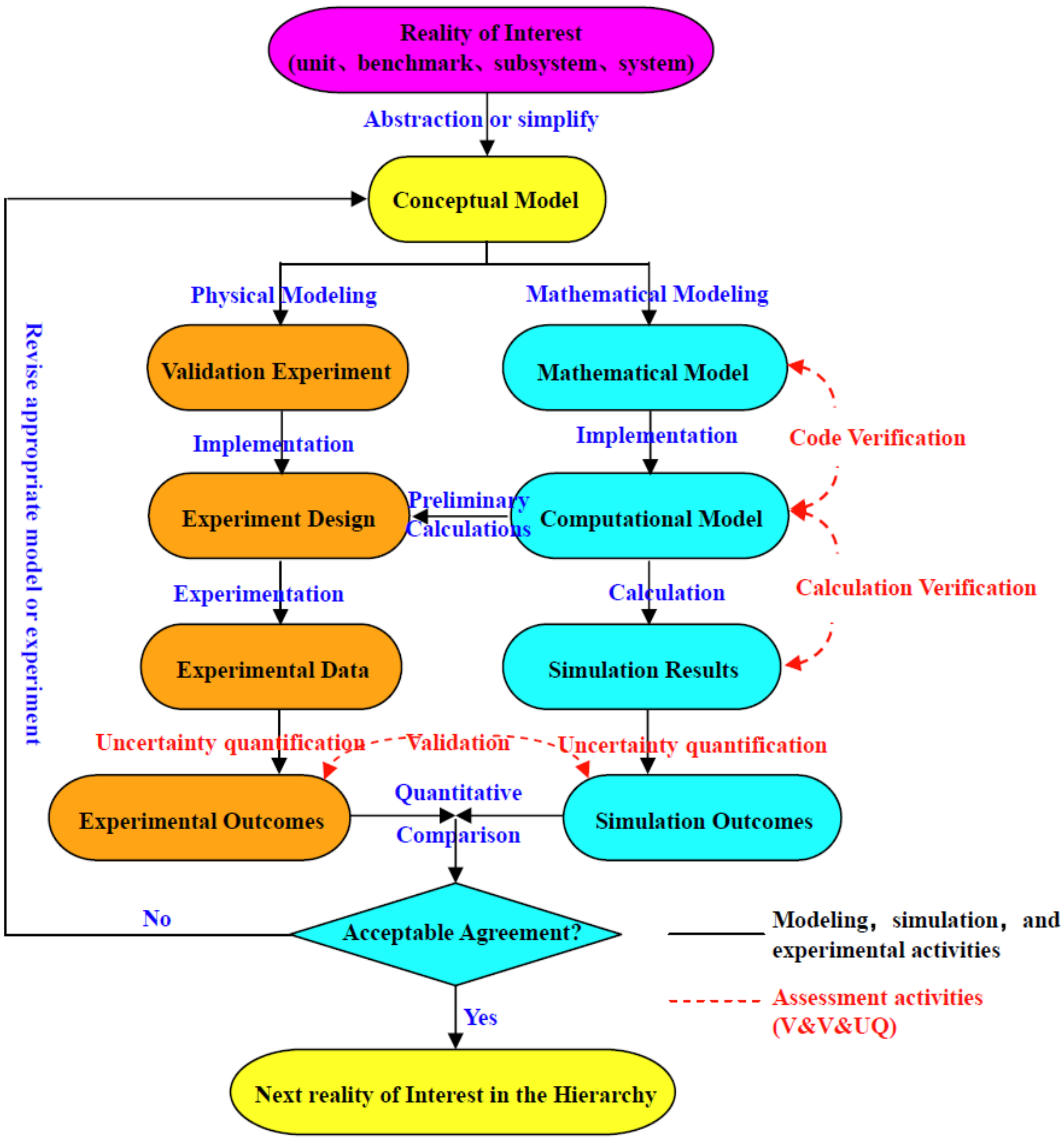

- Left figure presents the content and procedure of the V&V&UQ activity and model development. We can see that there are two branches (experiment, simulation) in the V&V for reality of interest.

- Basic activity of V&V&UQ includes code verification, calculation verification, model validation, uncertainty quantification.

The Detonation Model(1)

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- The 2D Euler equations in non-conservative form

$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$	Mass equation	(1)
$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) + \nabla P = 0$	Momentum equation	(2)
$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \vec{u}) + \nabla \cdot (P\vec{u}) = 0$	Energy equation	(3)
$P = \begin{cases} P(\rho, e) & Non\ explosive \\ P(\rho, e, F) & explosive \end{cases}$	Equation of state	(4)
$\frac{d\lambda}{dt} = F(\rho, e, \lambda)$	Explosive reaction rate	(5)

Where ρ denotes the density, $\vec{u} = (u, v)^T$ is the velocity, e is the specific internal energy and P is the pressure, $E = e + \frac{1}{2}\vec{u}\cdot\vec{u}$ is the total energy.

The Detonation Model(2)

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➢ Burn function for explosive

To account for the effect of combustion on detonation dynamics, the pressure in the high explosive regions is computed using

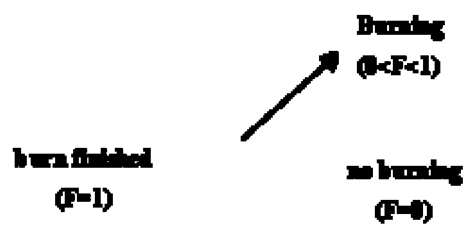
$$P = P_{EOS} \times F \qquad (7)$$

the burn fractions F that control the release of chemical energy are computed by

$$F = [\max(F_1, F_2)]^{n_2} \qquad (8)$$

Where $F=0$ denotes no burning; $0<F<1$ denotes burning; $F=1$ denotes burning finished。Wilkins function F_1 is:

$$F_1 = \begin{cases} 0, & V \ge V_0 \\ (V_0 - V)/(V_0 - V_J), & V_0 > V > V_J \\ 1, & V \le V_J \end{cases} \qquad (9)$$



C-J burn function F_2 is:

$$F_2 = \begin{cases} 0, & t \le t_b \\ (t - t_b)/\Delta L, & t_b < t < t_b + \Delta L \\ 1, & t \ge t_b + \Delta L \end{cases} \qquad (10)$$

where $V_J = \gamma V_0 / (\gamma + 1)$ denotes specific volume; V_0 denotes initial volume; γ denotes the ratio of specific heats for air; t is current time; t_b is the burn-beginning time; $\Delta L = r_b \Delta R / D_J$. ΔR is cell width; D_J is the detonation velocity; γ is the ratio of specific heats; n_b and Y_b are adjustable parameters.

The Detonation Model(3)

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- Equation of state for explosive

The Jones-Wilkins-Lee (JWL) equation of state (EOS) is used for the reacted and un- reacted gases in the explosive regions. The EOS of the pressure-dependent JWL type is

$$P_{EOS} = A\left(1-\frac{\omega}{R_1V}\right)e^{-R_1V} + B\left(1-\frac{\omega}{R_2V}\right)e^{-R_2V} + \frac{\omega E}{V} \qquad (6)$$

Where P_{EOS} is the pressure, V is relative specific volume, $V=\frac{\rho_0}{\rho}$, E is the detonation energy per unit volume, $E=\rho_0 e$, and A, B, R1, R2 and ω are constants to be calibrated. The calculated pressure of the shock wave by using JWL parameters determined by the numerical method agrees with experimental results.

- Equation of state for metal material

For a moderately realistic model, Mie-Grnneisen EOS has been used for the simulations of metal materials. It has following form:

$$P = \frac{\rho_0 C_0^2 \mu\left[1+\left(1-\frac{\gamma_0}{2}\right)\mu\right]}{\left[1-(S_\alpha-1)\mu\right]^2} + \gamma_0 E, \qquad \mu = \frac{\rho}{\rho_0} - 1 \qquad (7)$$

where C_0、S_α、γ_0 are the Grunneisen constants. ρ_0 denote the physical property parameters.

LAD2D Code (1)

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- The main features of LAD2D

LAD2D computer code, which numerically solves the equations of multi-material, compressible fluid dynamics. Of particular interest is the general capability to handle material interfaces, including slip, cavitations, or void closure. Also included is the capability to treat high explosive (HE).

- **LAD2D**: **L**agrange **A**daptive hydro**D**ynamics code in **T**wo **D**imensions
- Solve multi-material, large deformation elastic-plastic flows；
- Object-oriented programming ， generality, reliability and maintainability， good modification;
- Fortran 90 and C ++ programming language;
- LAD2D consists of the main body and several independent general modules。 The main body includes a control, a pre-process, a central operation, a grid, a post-process sub-systems, a common data module and a error process sub-system. The four independent general modules are grid generation(GRID2D), adaptive mesh refinement (AMR2D), remapping (REMAP2D) and grid adaption (ADAP2D) ;
- More than 200,000 line statements。

LAD2D Code (2)

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- The LAD2D code architecture (see Figure 1)

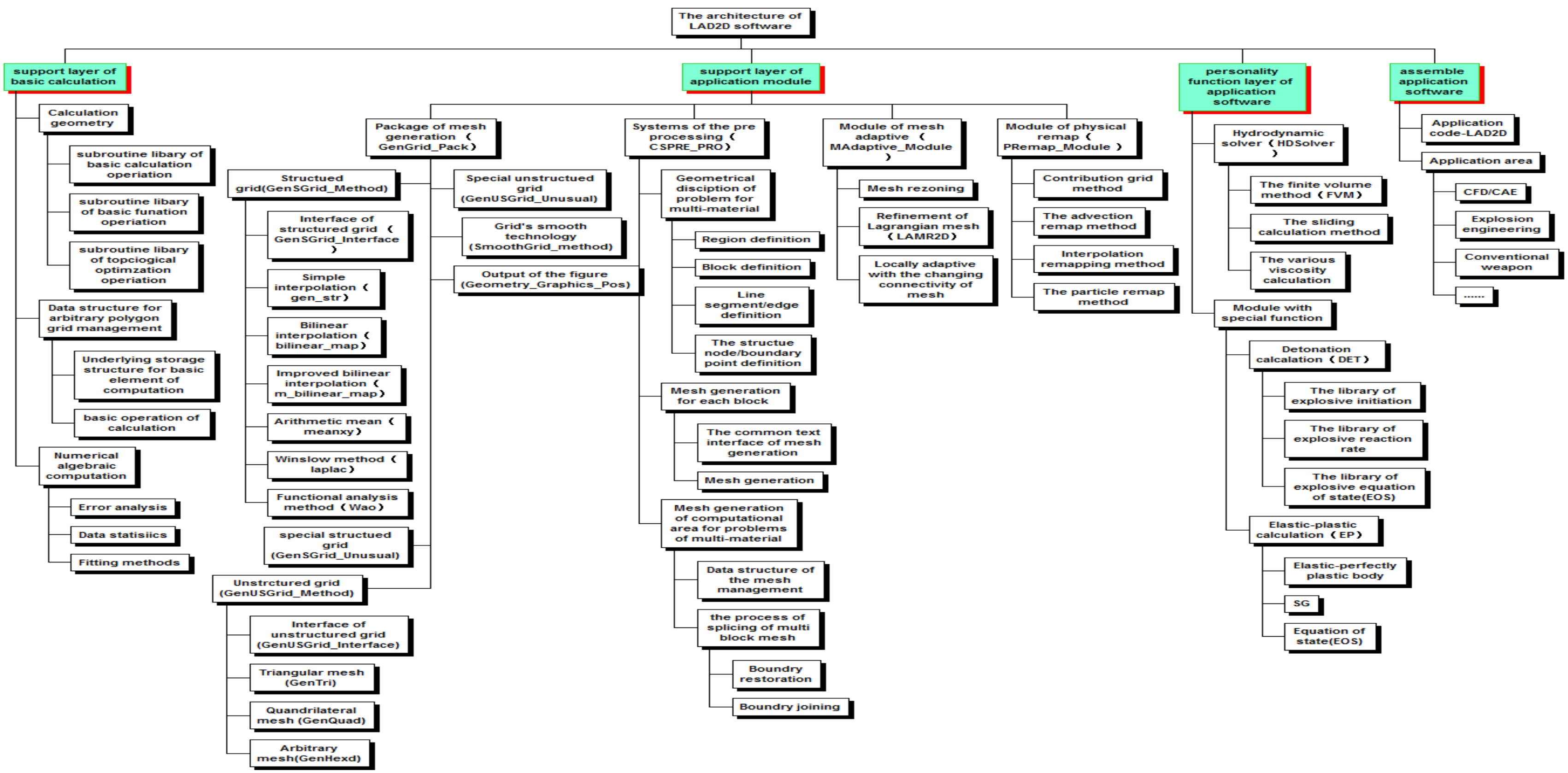

FIGURE 1. The LAD2D code architecture

Including: **1 support layer of basic calculation; 2 support layer of application module;**

3 personality function layer of application software; 4 assemble application software

LAD2D Code (3)

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➢ Computational scheme of LAD2D

The computational method is based on the arbitrary unstructured polygonal grid. The **Lagrangian finite volume method** and various viscosity such as classical Von Neumann-Richtmyer viscosity (the quadratic form viscosity), Landshoff viscosity (linear viscosity), shock wave viscosity, subzonal pressure method, artificial heat exchange in eliminating nonphysical deformation of Lagrangian mesh.

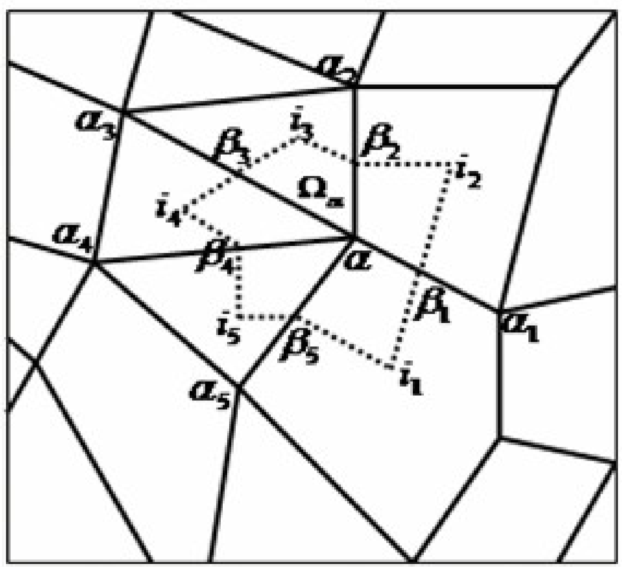

Fig.1 Control volume Ω_α of momentum equation

$$u_\alpha^{n+\frac{1}{2}} = u_\alpha^{n-\frac{1}{2}} + \frac{\Delta t^n}{B_\alpha^n}\sum_{k=1}^{m_\alpha^n}\left\{-\left[(p+q)^n_{\beta_{k-1},i_k}\left(r^n_{i_k} - r^n_{\beta_{k-1}}\right) + (p+q)^n_{i_k,\beta_k}\left(r^n_{\beta_k} - r^n_{i_k}\right)\right]\right\}$$

$$v_\alpha^{n+\frac{1}{2}} = v_\alpha^{n-\frac{1}{2}} + \frac{\Delta t^n}{B_\alpha^n}\sum_{k=1}^{m_\alpha^n}\left\{+\left[(p+q)^n_{\beta_{k-1},i_k}\left(x^n_{i_k} - x^n_{\beta_{k-1}}\right) + (p+q)^n_{i_k,\beta_k}\left(x^n_{\beta_k} - x^n_{i_k}\right)\right]\right\}$$

Where $B_\alpha^n = \sum_{k=1}^{m_\alpha^n} \frac{\rho^n_{i_k} A^n_{i_k}}{l^n_{i_k}}$, q is the artificial viscosity,

Δt is the time step, the subscript denotes the Lagrangian cell or vortex, the superscript refers to the iteration number, A is the area of the mesh.

LAD2D Code (4)

➤ The Changing Connectivity of Mesh Technology

The changing connectivity of mesh (topology transformation) is allowed during numerical simulation. Topological operations such as splitting and elimination of cells and edges, merging of cells is allowed in simulation process. This approach has successfully been implemented in LAD2D codes.

For example, figure 2 shows an example of a detonation wave behind a backward-facing step. The changing connectivity of mesh technology was used during the computational process.

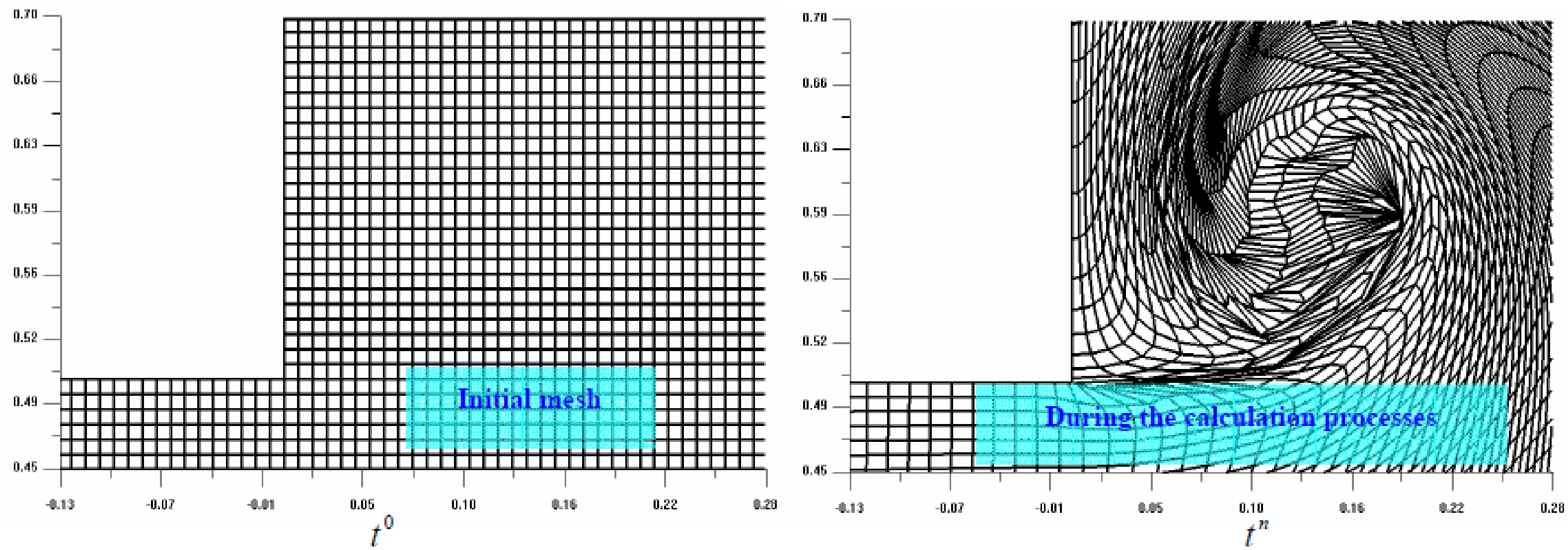

 FIGURE 2. The changing connectivity of mesh applies to handle the large deformation

V&V Strategy of LAD2D (1)

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- The figure 3 was presented the strategy for V&V&UQ of the detonation fluid dynamics in LAD2D.

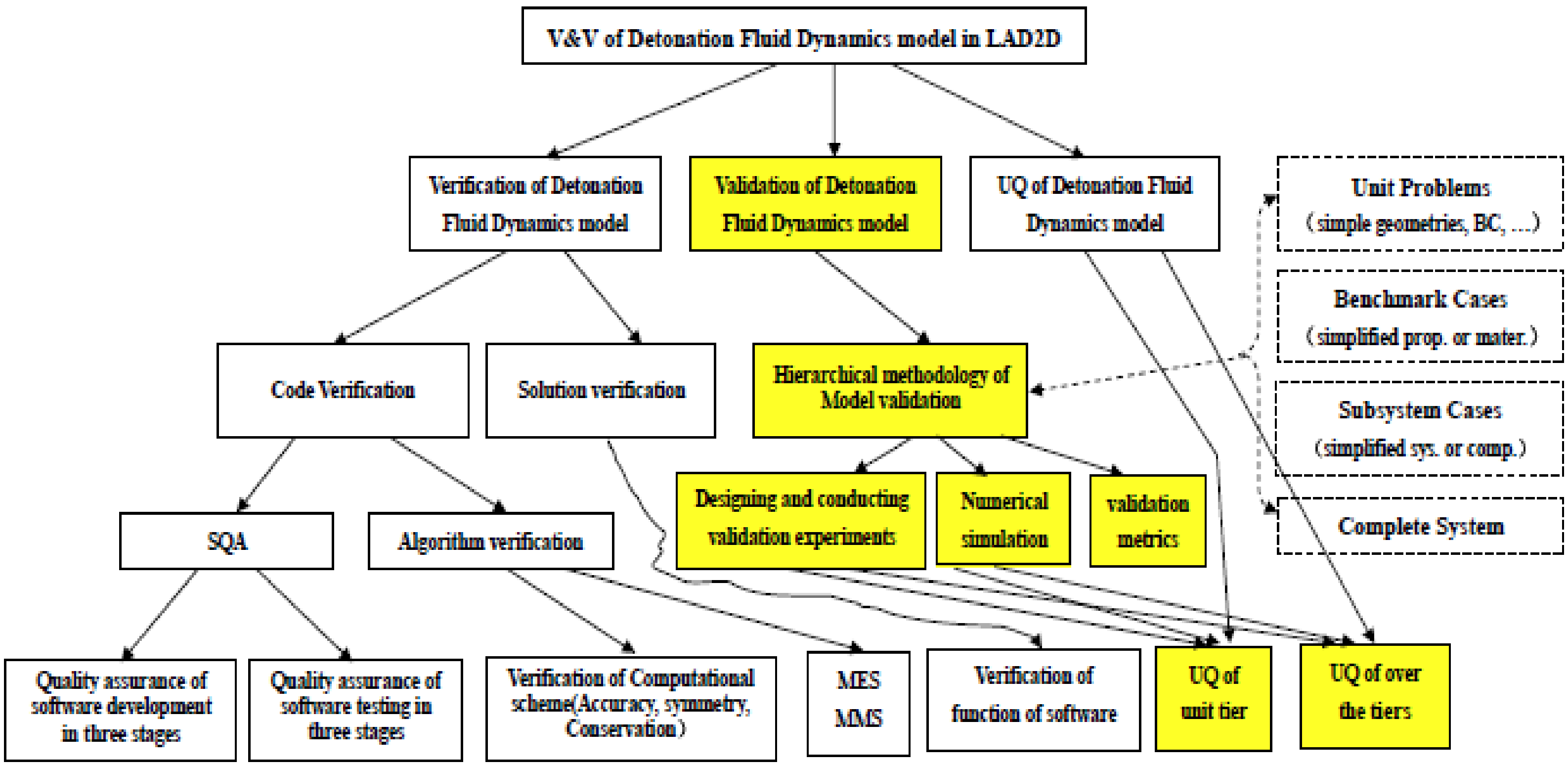

FIGURE 3. verification, validation and uncertainty quantification in LAD2D

From the upper layer to the lower layer, including type and content of the verification, validation and uncertainty quantification..

V&V Strategy of LAD2D (2)

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- Software Quality Assurance

The software quality assurance (SQA) is used to validate the quality of the software from software development to product release. We have suggested the software quality assurance model for development processes of 15 nodes of three stages based on the software engineering method. For detailed information, please see Figure 4.

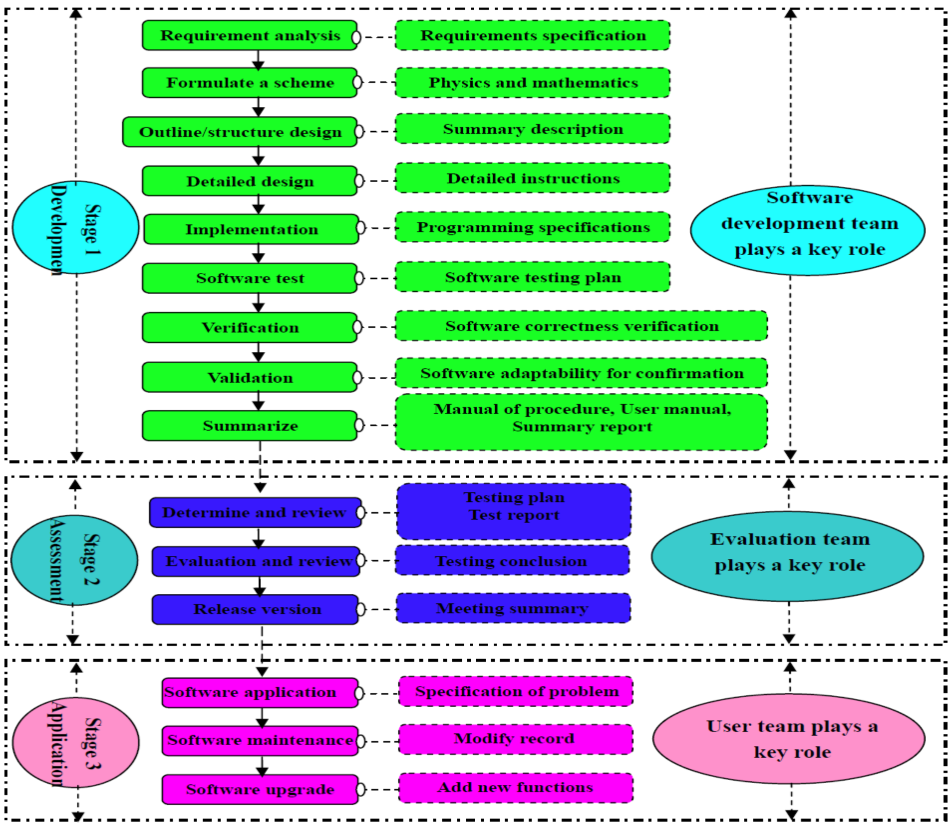

FIGURE 4. Quality assurance of software development in three stages

V&V Strategy of LAD2D (3)

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- Method of manufactured solutions

The method of manufactured solutions (MMS) is a more general approach for code verification. Contrast with the method of exact solution (MES), the MMS is more powerful in code verification within complex, nonlinear, higher dimensions, coupled PDEs. We have constructed MMS of hydrodynamics Euler equations in Lagrangian framework. The Figure 5 presents the procedure of MMS for code verification. Comparison between the numerical solutions and the MMS of time versus distance, velocity, density, pressure at versus initial position. The numerical solution is in good agreement with MMS.

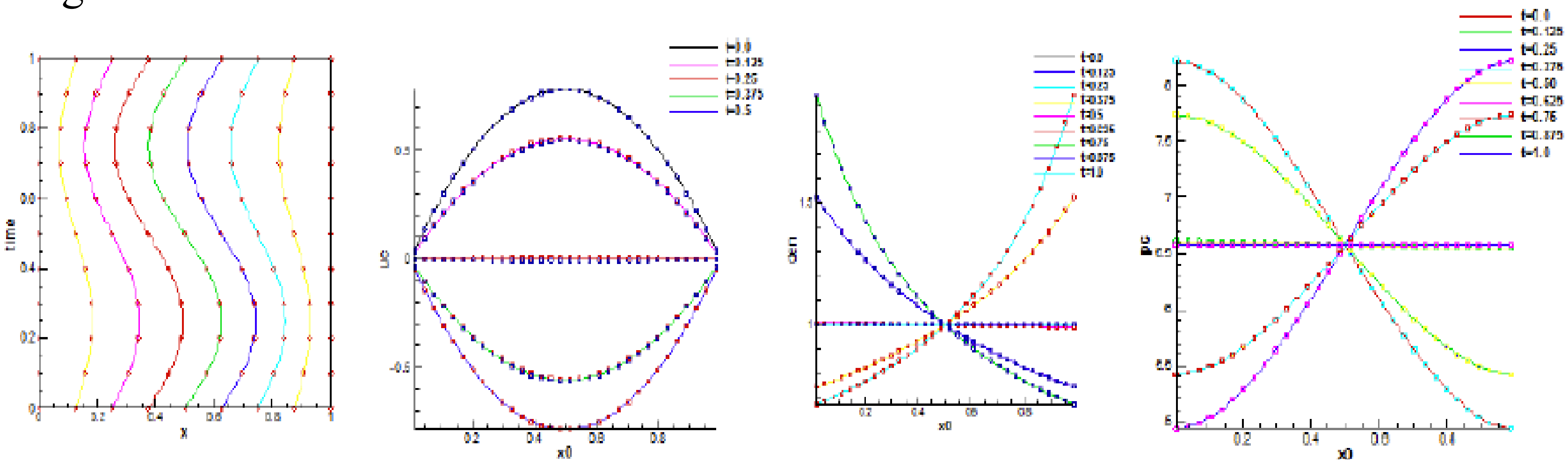

FIGURE 5. Comparison between the numerical solutions and the MMS of time versus distance, velocity, density, pressure versus initial position (Dashed line: numerical solution; Solid line: MMS)

V&V Strategy of LAD2D (4)

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- Validation experiment hierarchy

Validation experiment hierarchy approach is recommended in the complex physical coupling system when it is impossible and impractical to conduct the direct validation experiment on the complete system. We have been constructed the validation hierarchy tiers of the detonation fluid dynamics model in LAD2D. For detailed information about validation activity of explosive detonation, please see Figure 6.

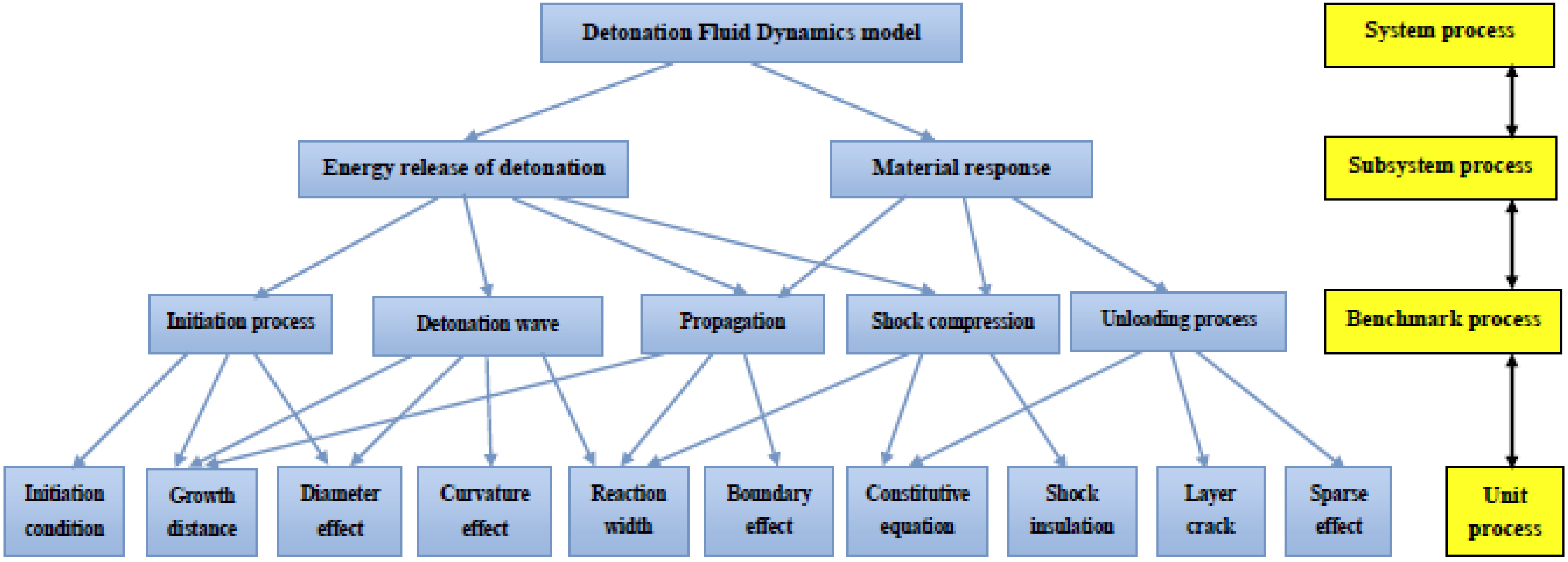

FIGURE 6. Validation hierarchy tiers of the detonation fluid dynamics model

V&V Strategy of LAD2D (5)

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➢ UQ and predictive capabilities

- we propose an efficient development assessment process for predictive software with high confidence (see figure 7). The best choice for the uncertainty quantification of any specific code will depends on experiments.

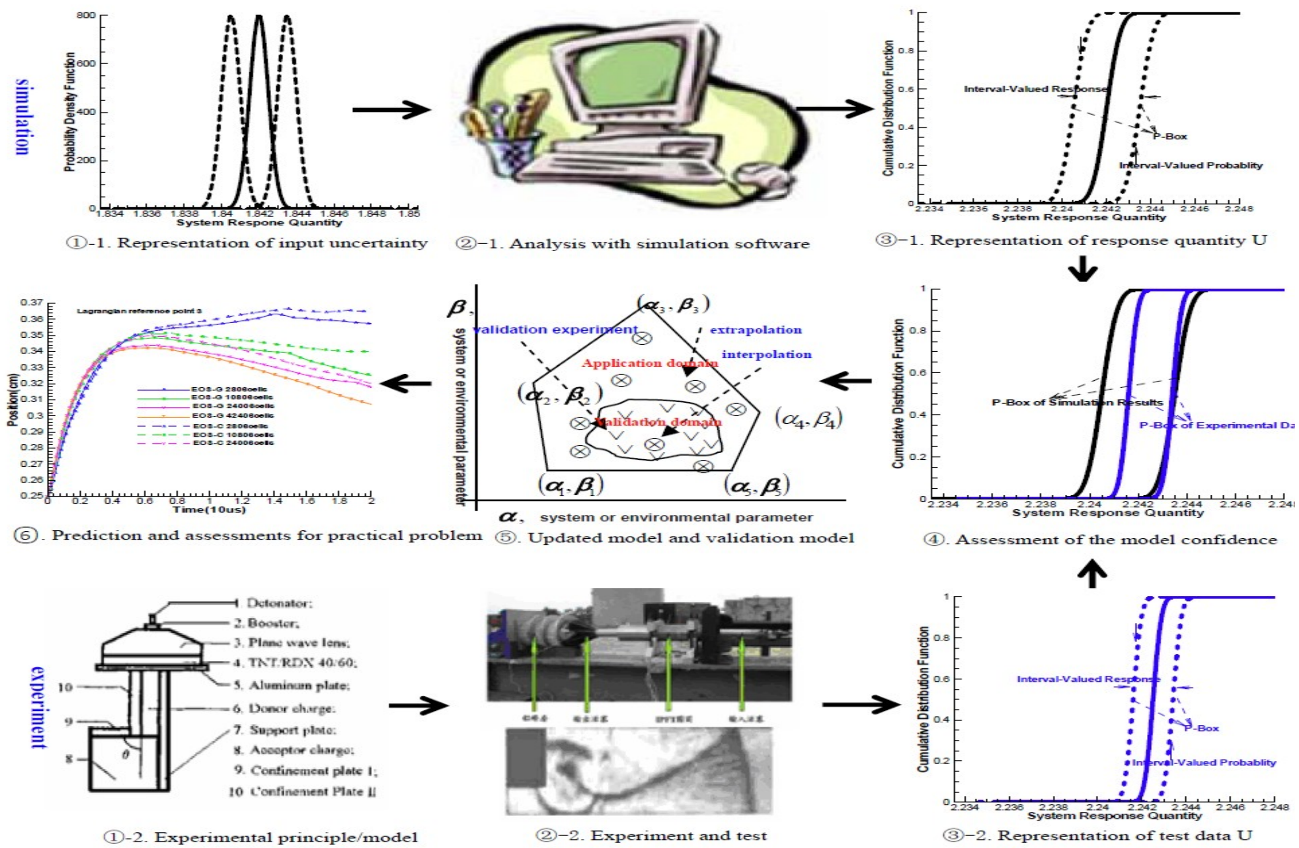

FIGURE 7. The assessment process for predictive software with high confidence

Parts of Result of V&V(1)

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➢ Precision verification

The one-dimensional (1D) Riemann problem used in code tests is widely known as Sod's problem. Here is an example using blast wave problems. Blast wave problems are generally computational domain [-1,1] the initial value:

$$\begin{cases} \rho_L = 1.4 \\ U_L = -2.6 \\ P_L = 37.1765 \\ \gamma_L = 1.4 \end{cases} x \le 0 \; ; \quad \begin{cases} \rho_R = 15.293 \\ U_R = 0.0 \\ P_R = 1.0 \\ \gamma_R = 3.1 \end{cases} x > 0$$

Figure 8 shows numerical results with 14 sets of 50 to 900 mesh (50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900) . we can see LAD2D procedures in the calculation of the problem of strong shock waves, with the encryption of the grid, the numerical solution gradually approaching the analytical solution

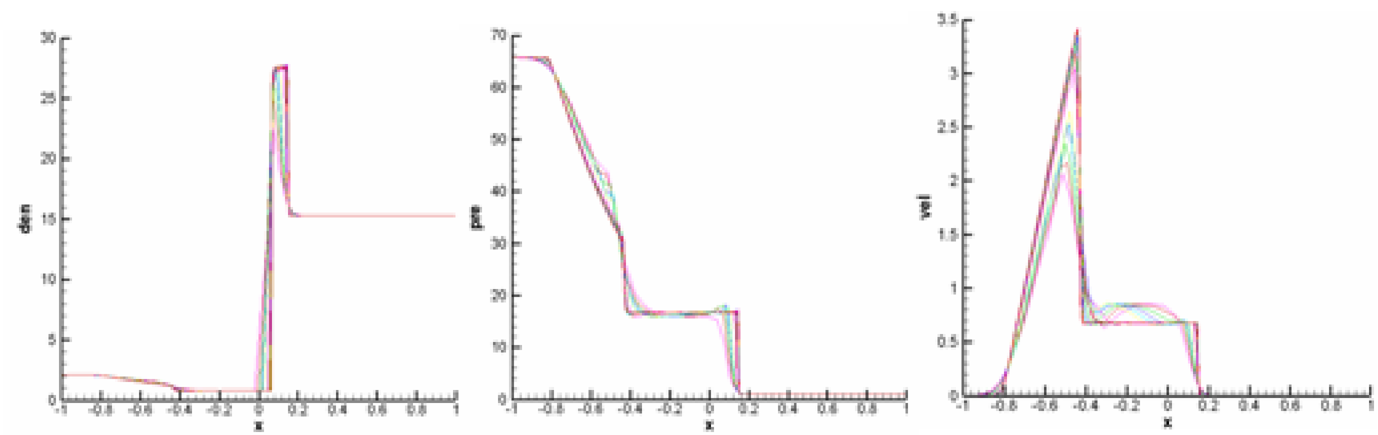

Figure 8 Comparison between numerical results with the analytical solution for grid scale from 0.04 to 0.025

Parts of Result of V&V(2)

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➢ Model validation-Experiment model

Here is a example using Diffraction of a detonation wave behind a backward-facing step. This problem models is a detonation wave propagating through the channels with suddenly expending section(see Figure 9). The left is a little section channels, the right region is a large section channels. The computational domain is Ω as described in figure 10. Ω is split into two regions filled with the explosive PBX-9404 with parameters K=2.996, $D_J = 8.88 \,{}^{km}\!/_{s}$, $\rho_0 = 1.84 \,{}^{g}\!/_{cm^3}$. The left region is $\Omega_1 = [0;3.0] \times [0;0.5]$, The right region is $\Omega_2 = [3.0;6.0] \times [0;3.0]$. The driver section is in the left part of the Ω_1, the upper boundary is a solid-wall condition, The lower is a axisymmetric condition The parameters A, B, R1, R2 and ω for JWL are $A = 8.524$, $B = 0.1802$, $R_1 = 4.6$, $R_2 = 1.3$, $w = 0.38$. The parameters n_b and γ_b are$n_b = 1.1$, $\gamma_b = 2.1$.

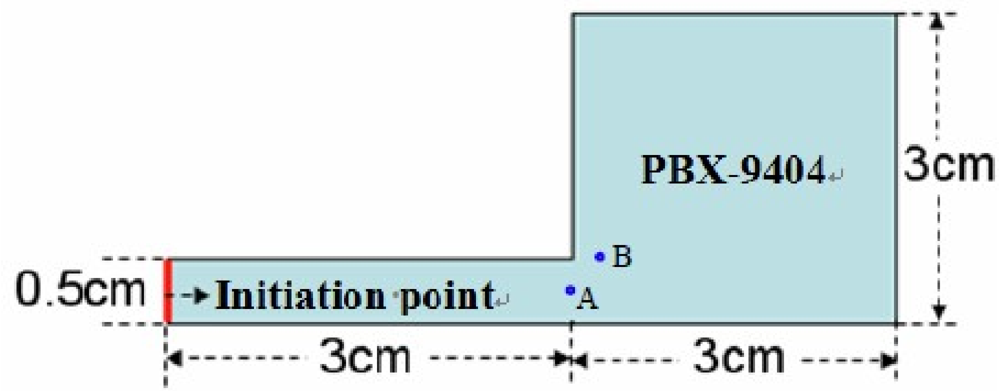
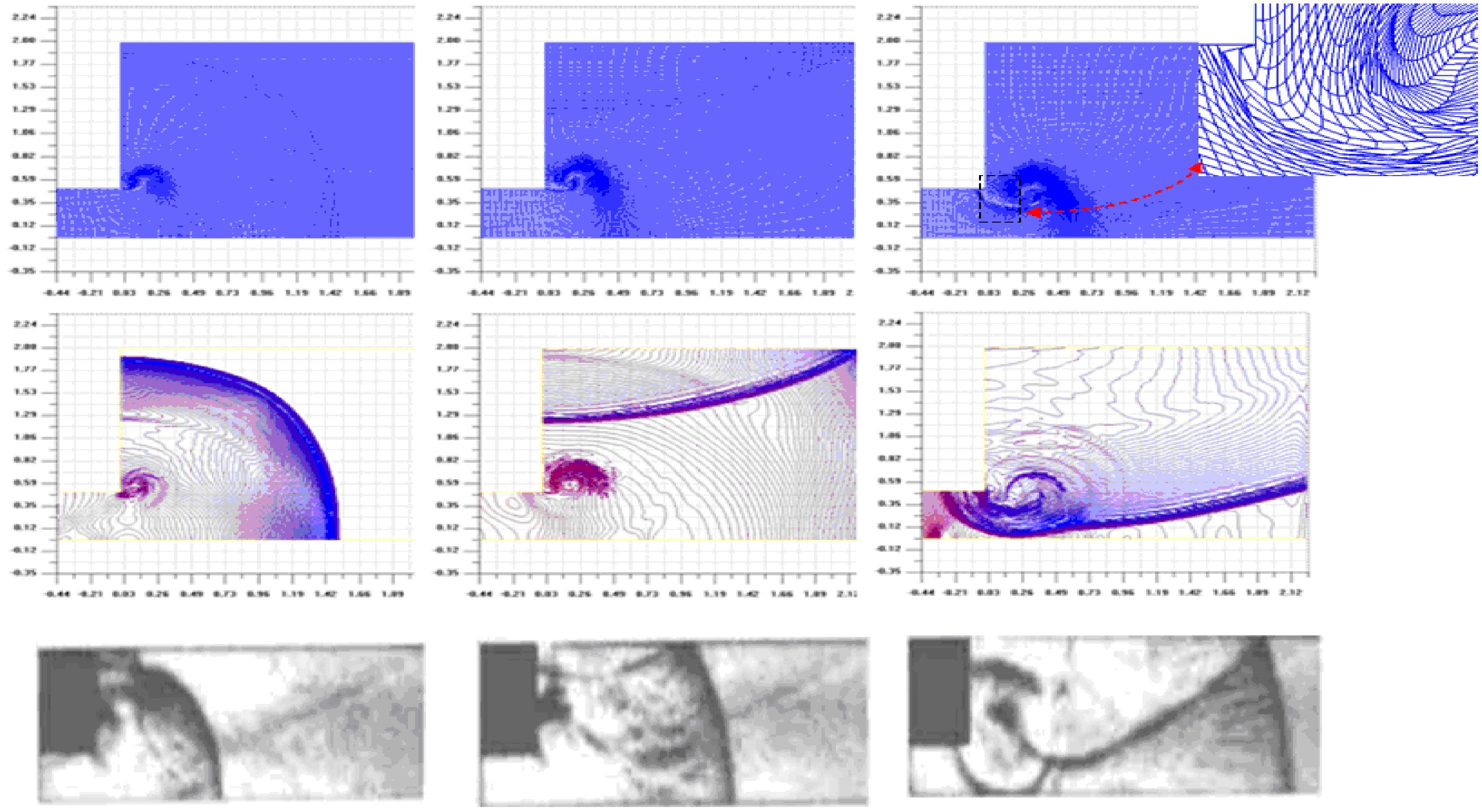


Figure 9 Computational domain for detonation wave behind a backward-facing steps, and in near corner containing Lagrangian reference point A and point B.

Parts of Result of V&V(3)

Figure 10 shows the computing mesh (upper) and density contours (lower) at three times. Diffraction through the 90^0 corner also generates a stronger corner vortex. We compare numerical results with experimental data by using high-speed schlieren photography, which coincide qualitatively.

Validation of the numerical simulation



Comparison between numerical results with the experimental data, LAD2D software is reliable.

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Parts of Result of V&V(4)

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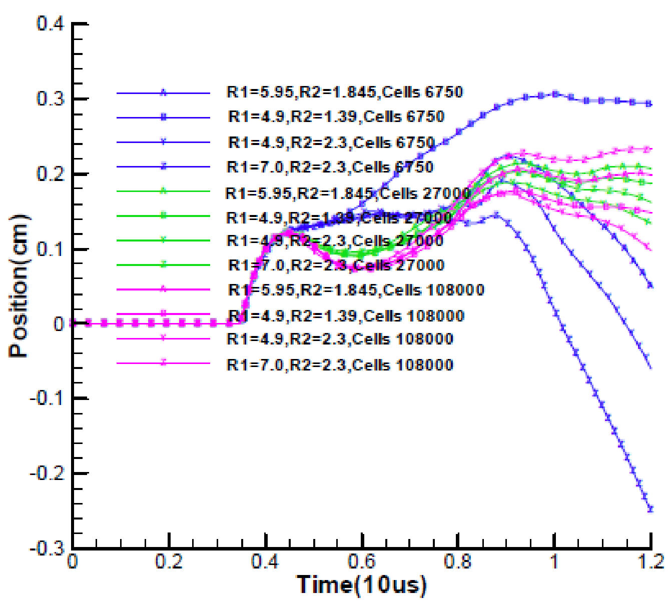
➢Uncertainty quantification

In order to assessment numerical simulation capability to predict actual physical phenomenon, Figure 11 shows time histories for diffraction of a detonation wave behind a backward-facing step simulation, recorded position and velocity at Lagrangian reference point-A.



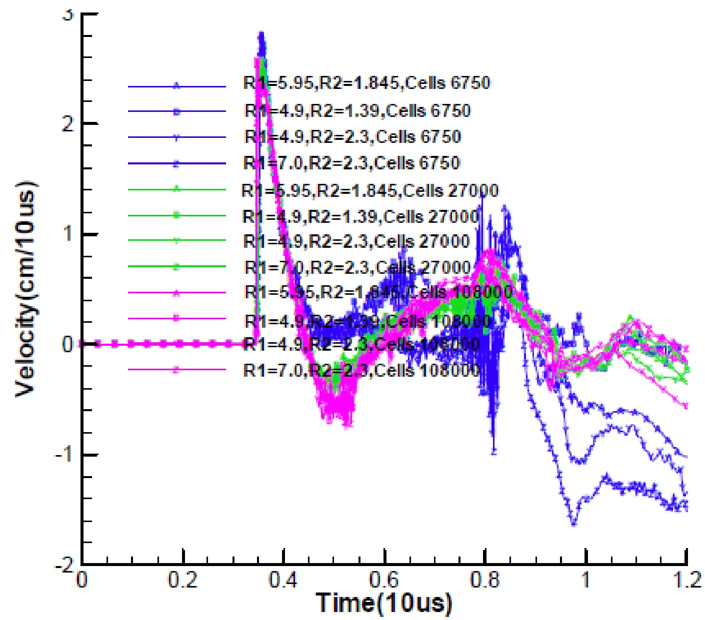


Figure 11 Time histories for diffraction of a detonation wave behind a backward-facing step simulation, recorded at Lagrangian reference point-A within 0.466667cm of the corner. The left is the position, the right is the velocity

Parts of Result of V&V(5)

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➢ Uncertainty quantification

Figure 12 shows time histories for diffraction of a detonation wave behind a backward-facing step simulation, recorded position and velocity at Lagrangian reference point-B.

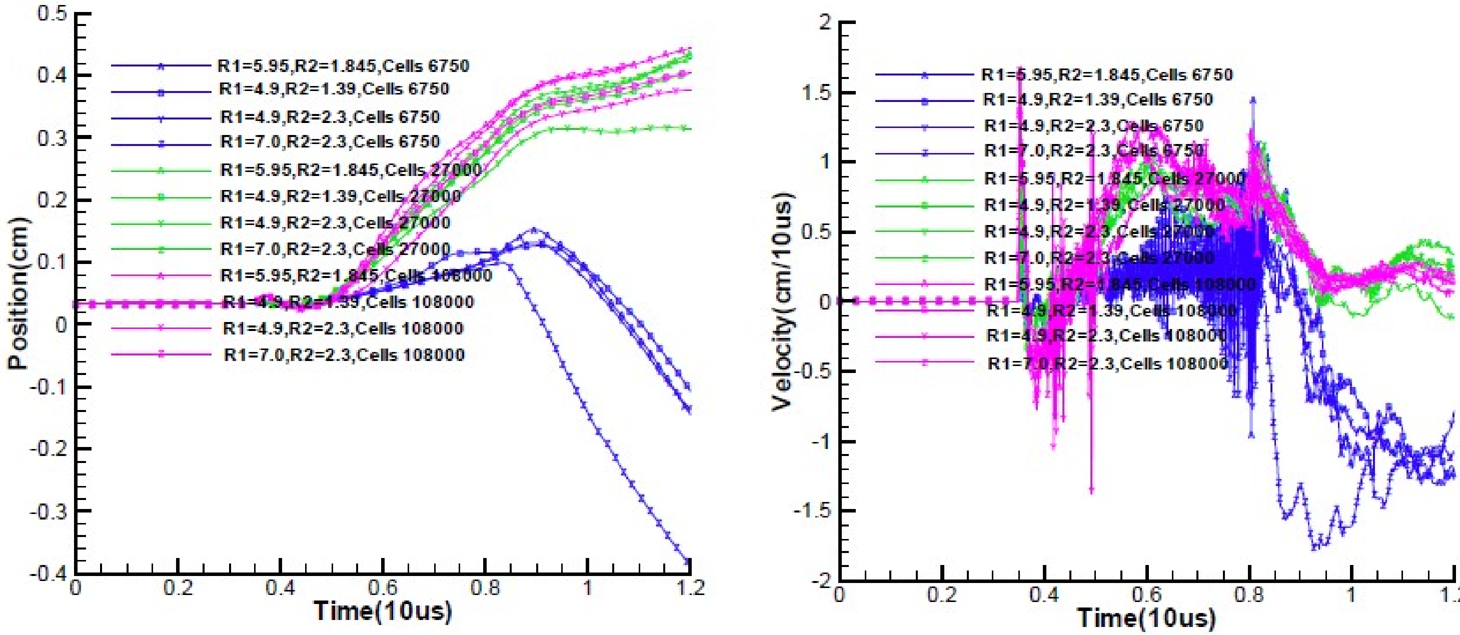

Figure 12 Time histories for diffraction of a detonation wave behind a backward-facing step simulation, recorded at Lagrangian reference point-A within 0.03333cm of the corner. The left is the position, the right is the velocity

Conclusion and Suggestions

- The credibility of the simulation results or prediction results in the numerical simulation software has an important influence on decision-making. Engineering application software V&V&UQ is a critical method used for evaluating the credibility of the software and simulation results.
- In this paper, we proposed the V&V&UQ strategy of detonation fluid dynamics LAD2D code. The V&V&UQ combines the strength of the physical experiment and numerical simulation; it is used to develop higher fidelity simulation software.
- The V&V&UQ strategy of detonation fluid dynamics in LAD2D was presents based on the foundation of scientific software's V&V method. The basic framework of the module verification methods and the function validation method were proposed.

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Thank you !