LSTC
Livermore Software Technology Corp.

Compressible CFD (CESE) Module Presentation

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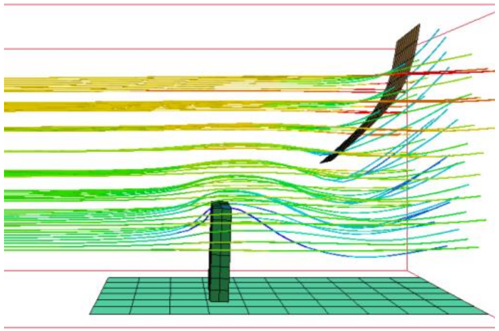
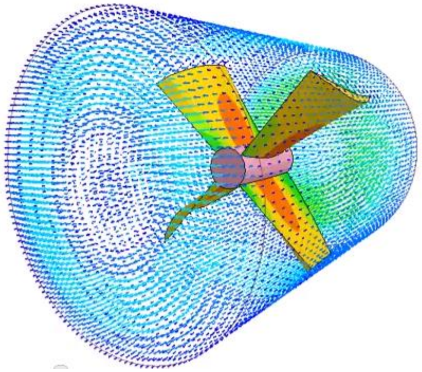
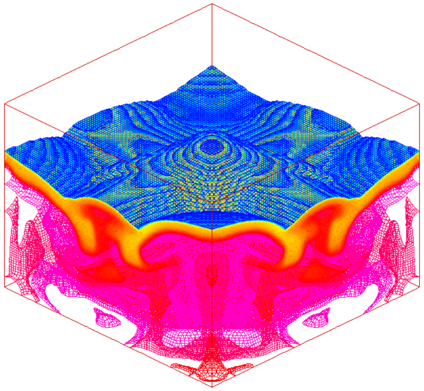
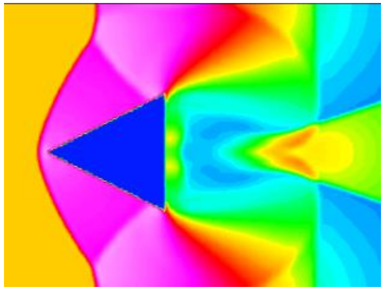

Introduction

1.1 Background

1.2 Main characteristics and features

1.3 Examples of applications

Background

LS-DYNA® is a **general-purpose** finite element program capable of simulating complex real world problems. It is used by the **automobile**, **aerospace**, **construction**, **military**, manufacturing, and bioengineering industries. LS-DYNA® is optimized for shared and distributed memory Unix, Linux, and Windows based, platforms, and it is fully QA'd by LSTC. The code's origins lie in **highly nonlinear, transient dynamic finite element analysis** using **explicit time integration**.

Some of LS-DYNA® main functionalities include:

- Full **2D** and **3D** capacities
- **Explicit/Implicit** mechanical solver
- Coupled **thermal** solver
- Specific methods: **SPH, ALE, EFG,** …
- **SMP** and **MPP** versions

- The new release version pursues the objective of LS-DYNA® to become a strongly coupled **multi-physics solver** capable of solving complex real world problems that include several domains of physics
- Three main new solvers will be introduced. Two fluid solvers for both **compressible flows (CESE solver)** and incompressible flows (ICFD solver) and the Electromagnetism solver (EM)
- This presentation will focus on the CESE solver
- The **scope** of these solvers is not only to solve their particular equations linked to their respective domains but to fully make use of LS-DYNA® capabilities by **coupling** them with the existing **structural** and/or **thermal** solvers

Introduction

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Main characteristics and features

- Double precision
- Second order explicit
- **2D and 2D axisymmetric** solver / **3D** solver
- FSI available for 3D solver
- **SMP** and **MPP** versions available
- Dynamic memory handling
- New set of keywords starting with ***CESE** for the solver
- **Automatically coupled** with LS-DYNA solid and thermal solvers
- Coupled with the R7 chemistry and stochastic particle solver (*CHEM and *STOCHASTIC)

CESE method main advantages

- A **unified treatment of space and time**

  (By the introduction of **conservation element** (CE) and **solution element** (SE), the conservation of scheme is always maintained in space and time, locally and globally)

- A **novel shock capturing strategy** without using a Riemann solver

- **High accuracy**

  (Both flow variables and its spatial derivatives are solved simultaneously)

Main features and applications

- **Highly accurate shock wave capturing**
  for compressible (M>0.3) and
  high speed supersonic flows (M>1)
- **Cavitation** model
- **Conjugate heat transfer** problems
- Many different kinds of **stochastic particle flows,**
  e.g, dust, water, fuel
- **Chemically reacting flows,**
  e.g, **detonating flow, supersonic combustion**

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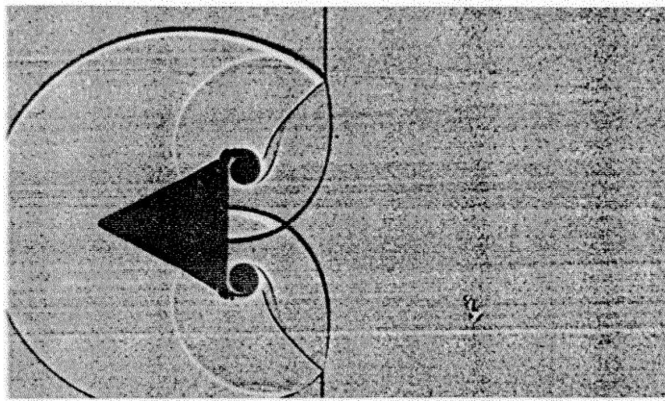
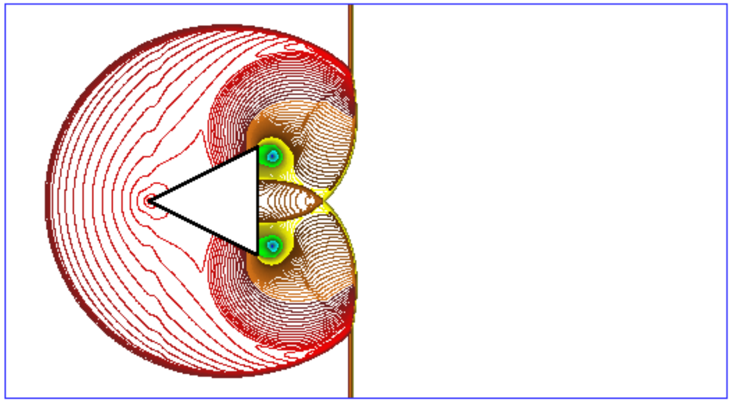
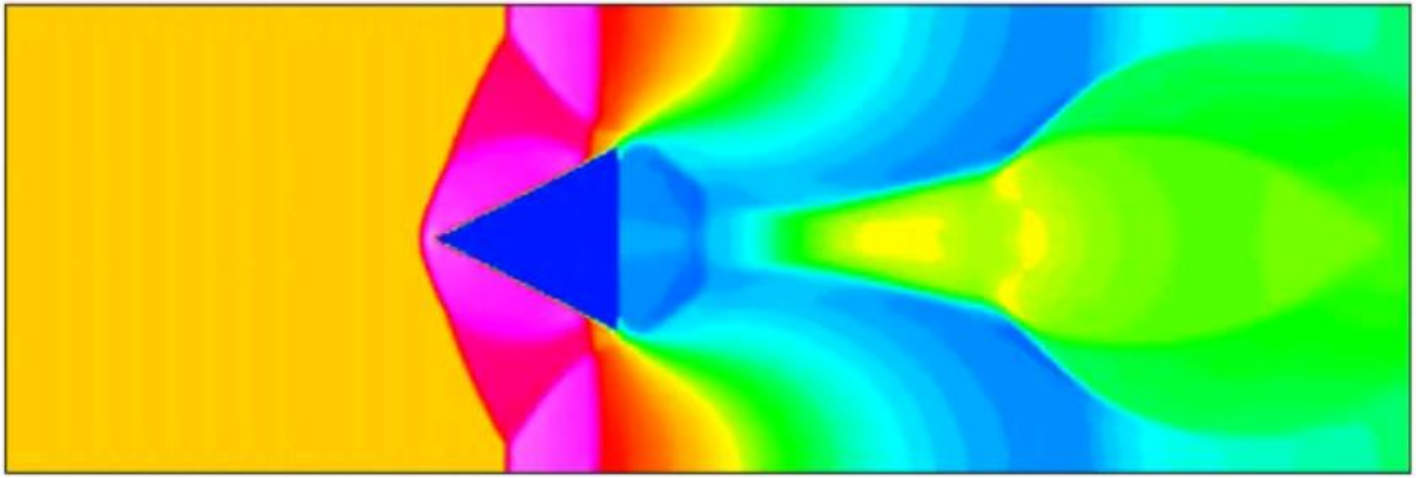
Supersonic shock wave capturing:

Experimental picture:

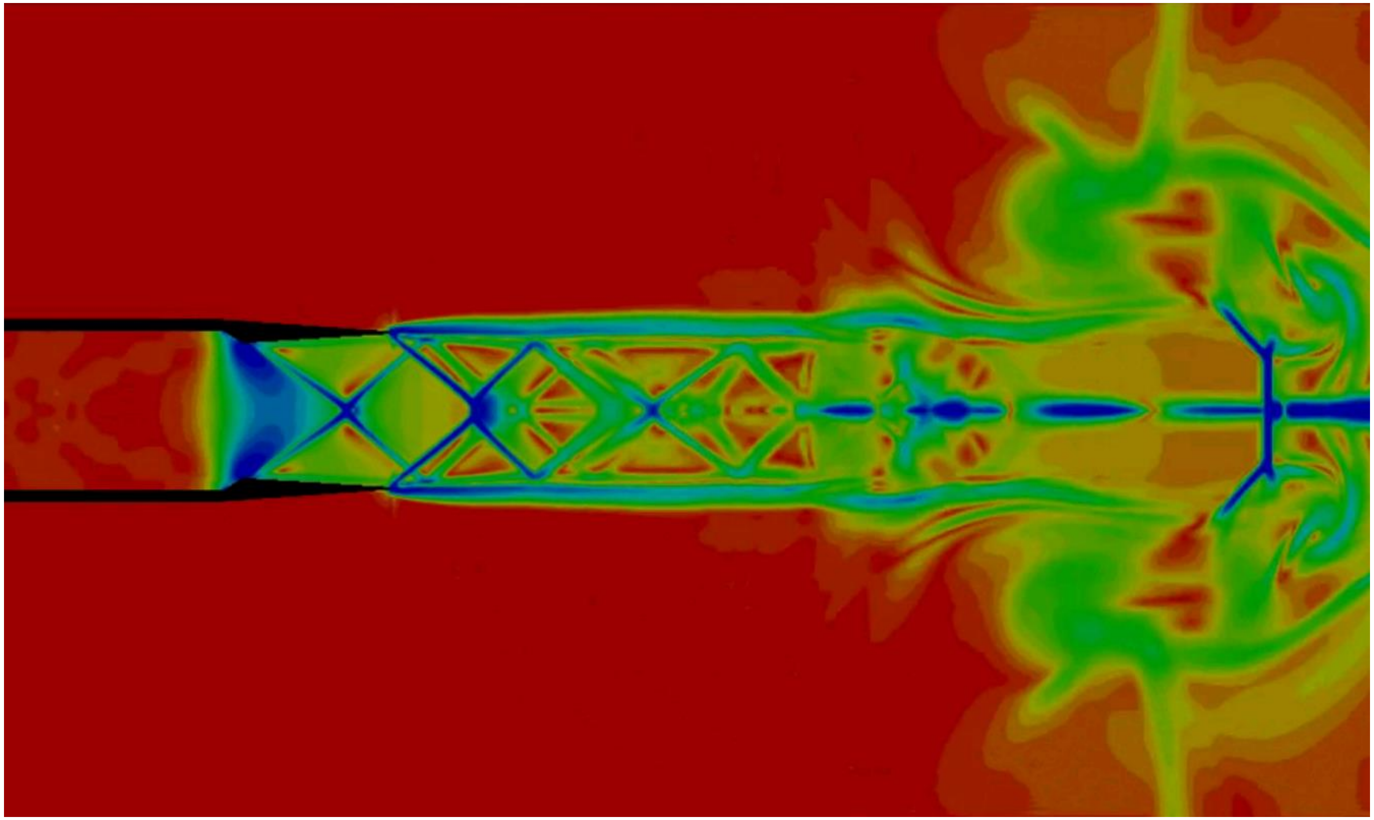


Numerical result:



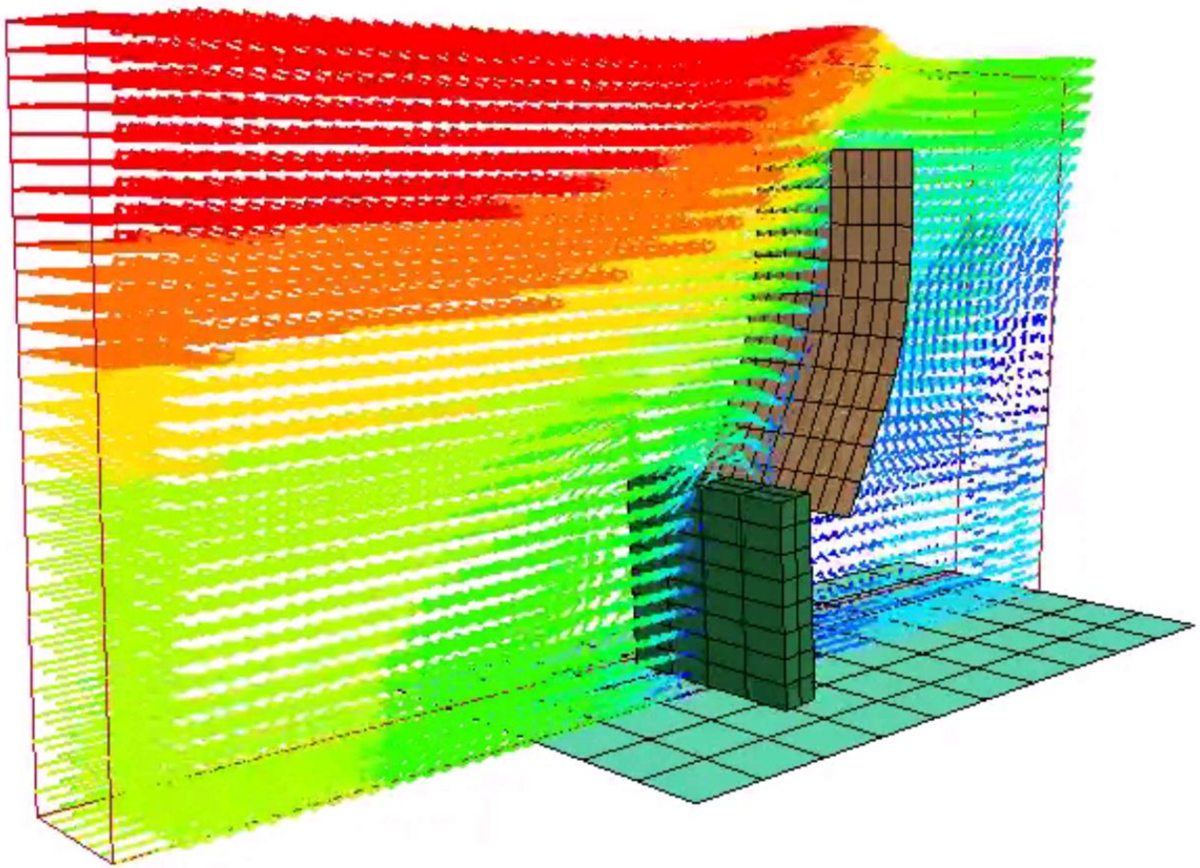


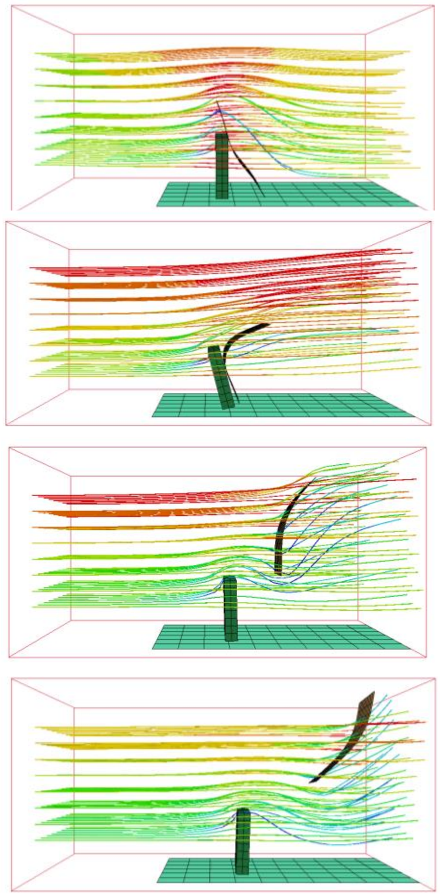
Flow structure of supersonic jets from conical nozzles (shock diamonds):



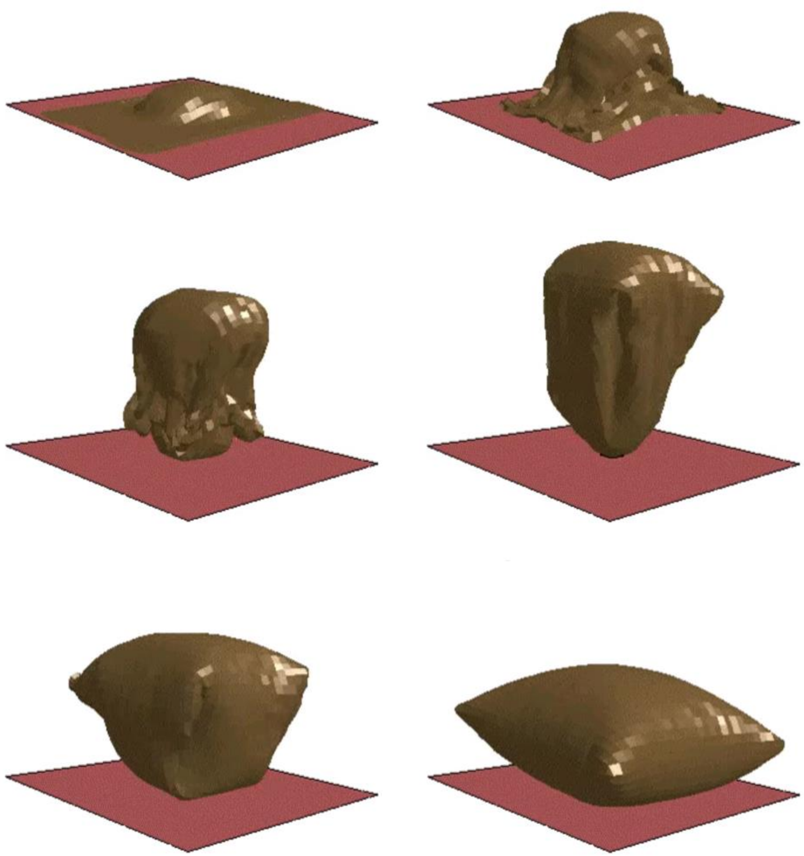
Courtesy of Kazuya Yamauchi Lancemore Corp., Japan

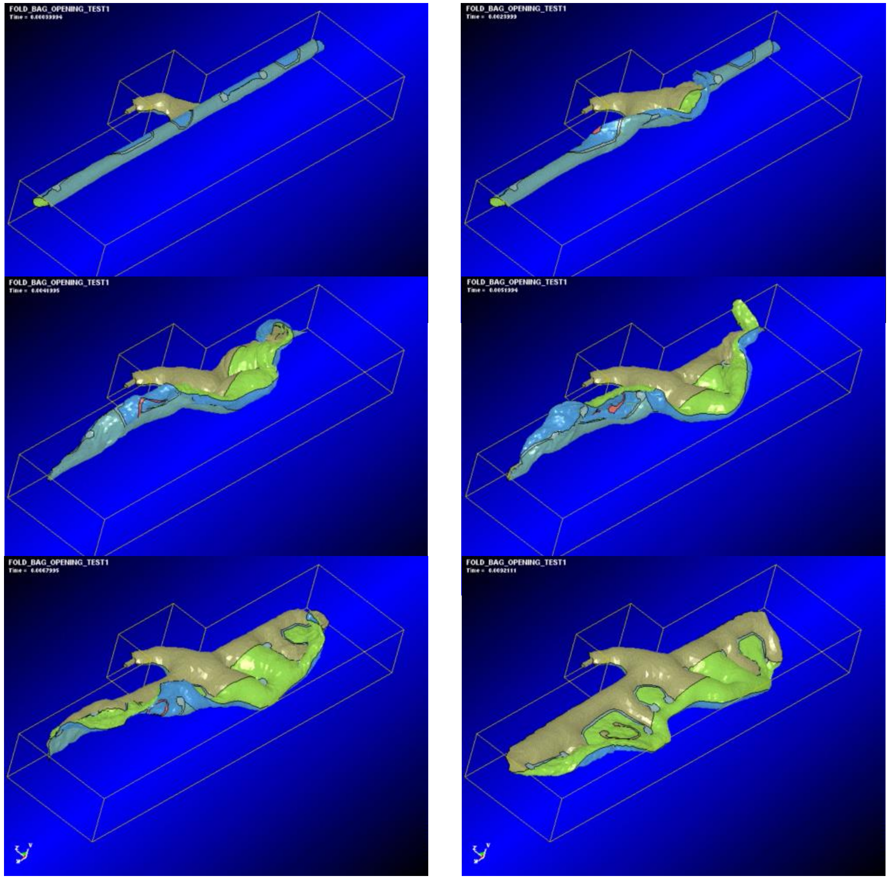
3D FSI waving flag problem:





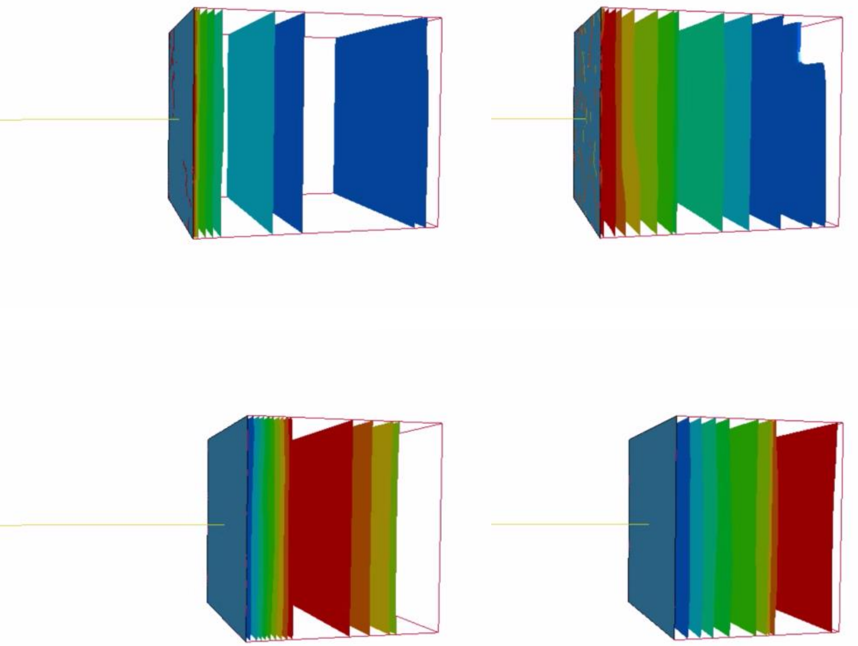
Airbag applications:



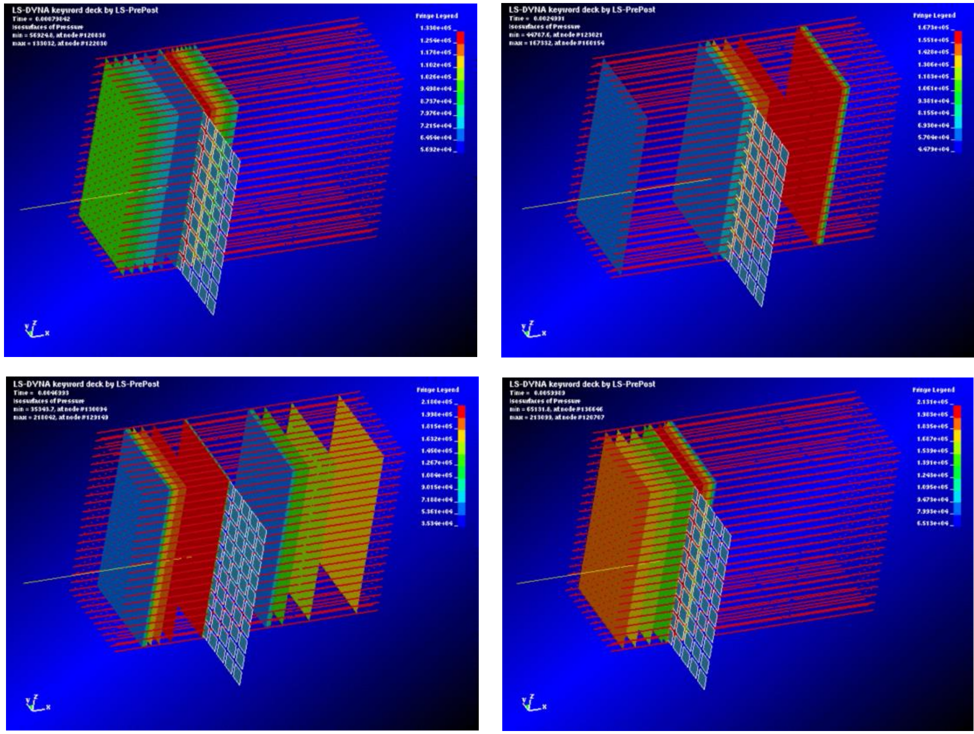


Courtesy of TAKATA Corp., Japan

Piston type applications with or without moving mesh:

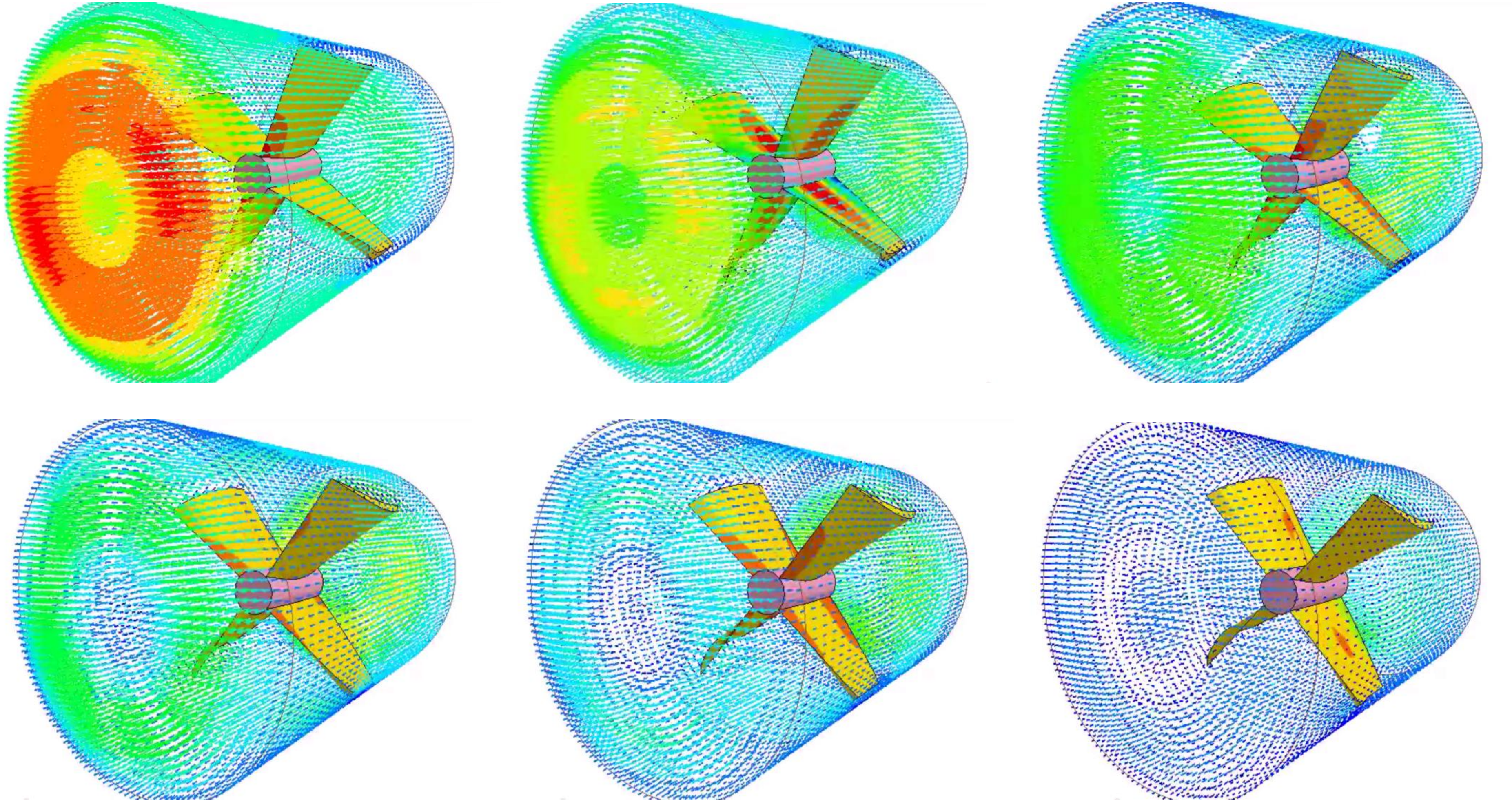


Moving mesh



Embedded mesh

Turbomachinery applications:



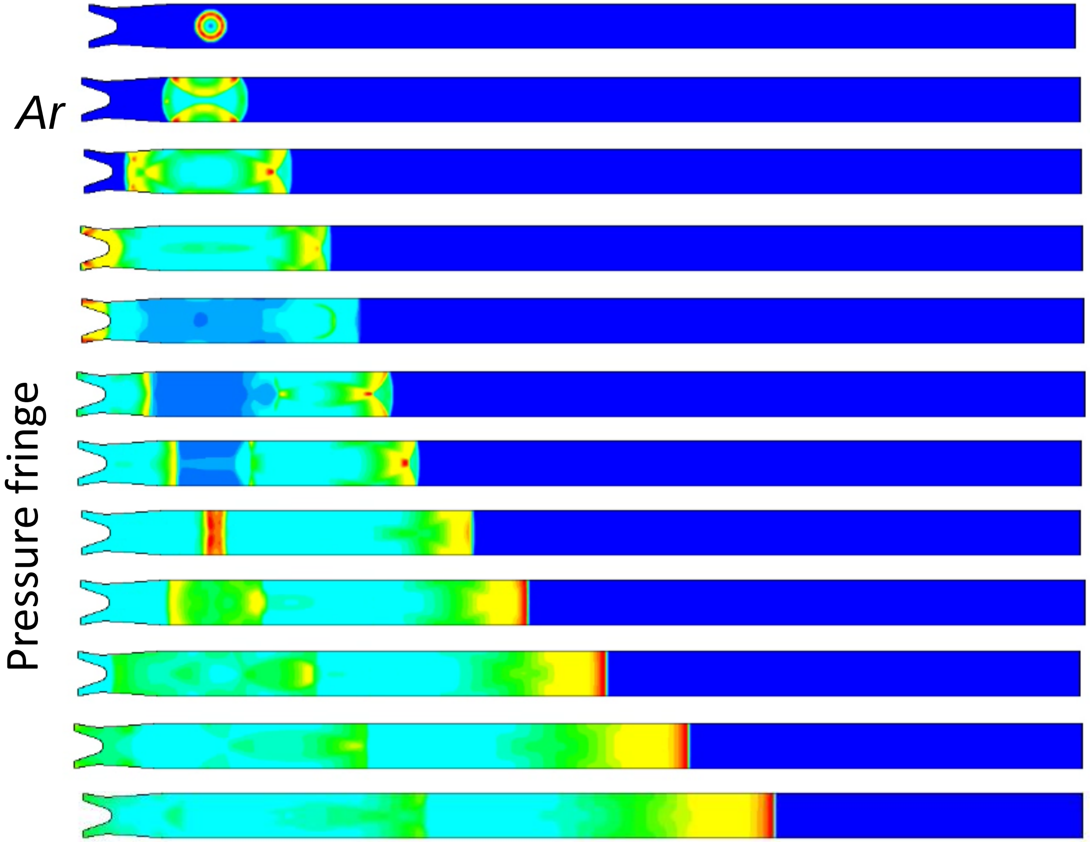
Detonation and chemical reactions:

Detailed reaction – realistic chemistry model

9 species:
H_2, O_2, H, H_2O, OH, O, HO_2, H_2O_2, Ar
with 18 reaction steps

Initial mixture:
$2H_2 + O_2 + 7Ar$
Euler equation

Courtesy Dr. R. Rosario
Bristol, U.K.



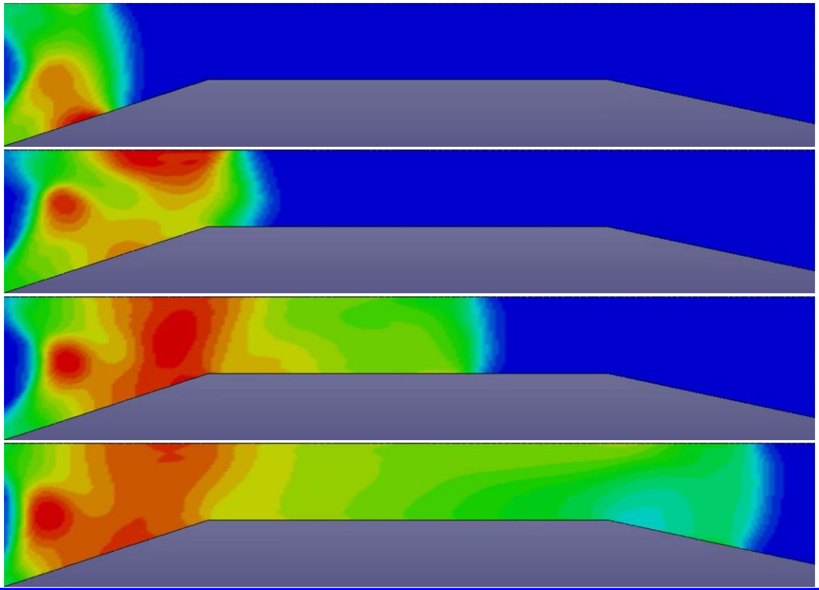
Chemical reactions at hypersonic speeds:

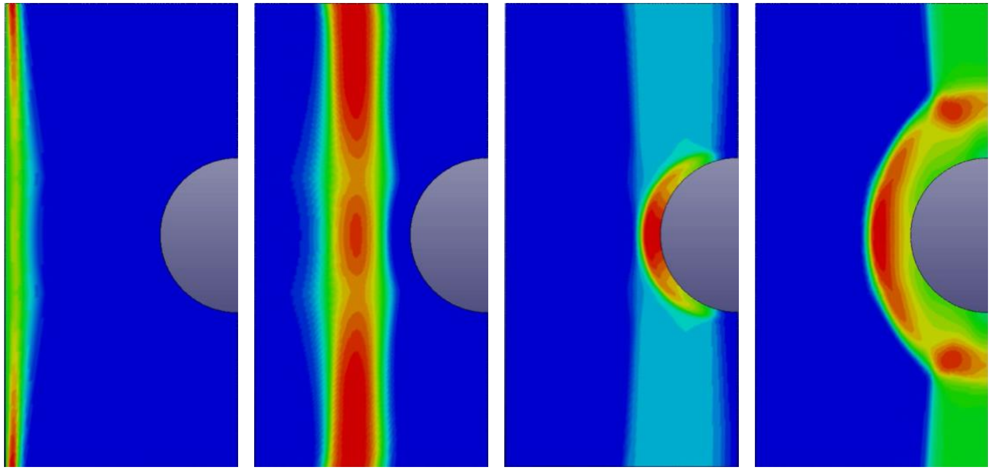
Detailed reaction model

5 species: O_2, N_2, O, N, NO
with 11 reaction steps

Initial mixture: $O_2 + 3.76N_2$

Navier-Stokes solver:



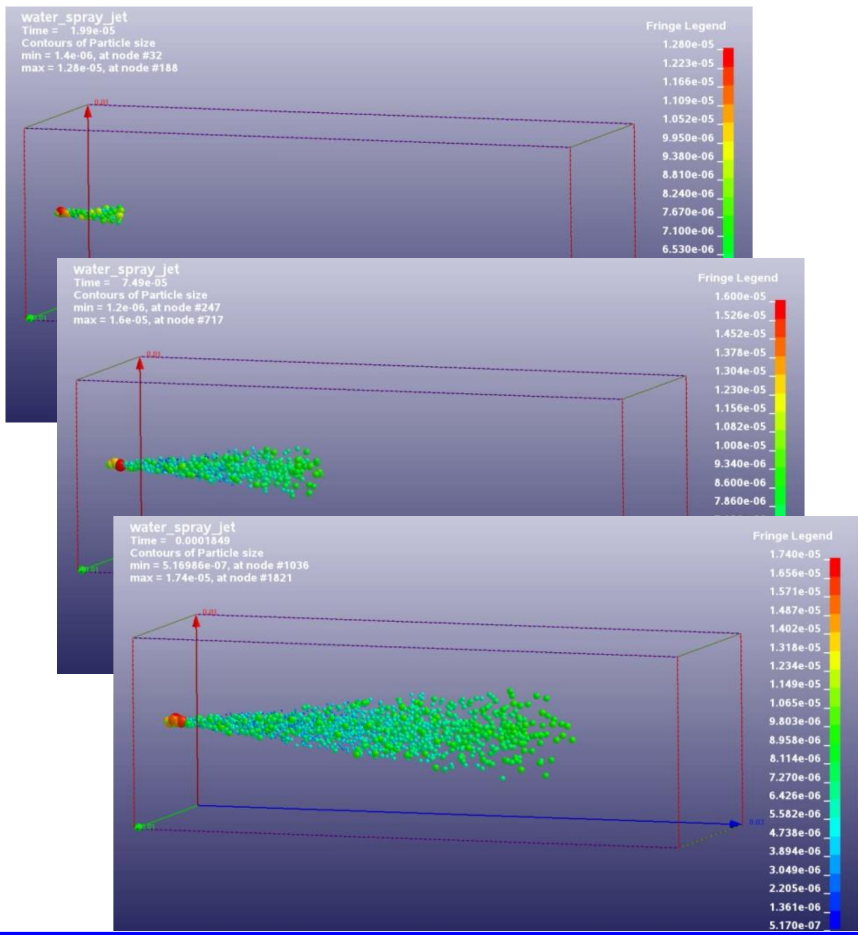


Pressure fringe of a blunt body:
Hypersonic inflow at Ma = 7 & T = 600 K

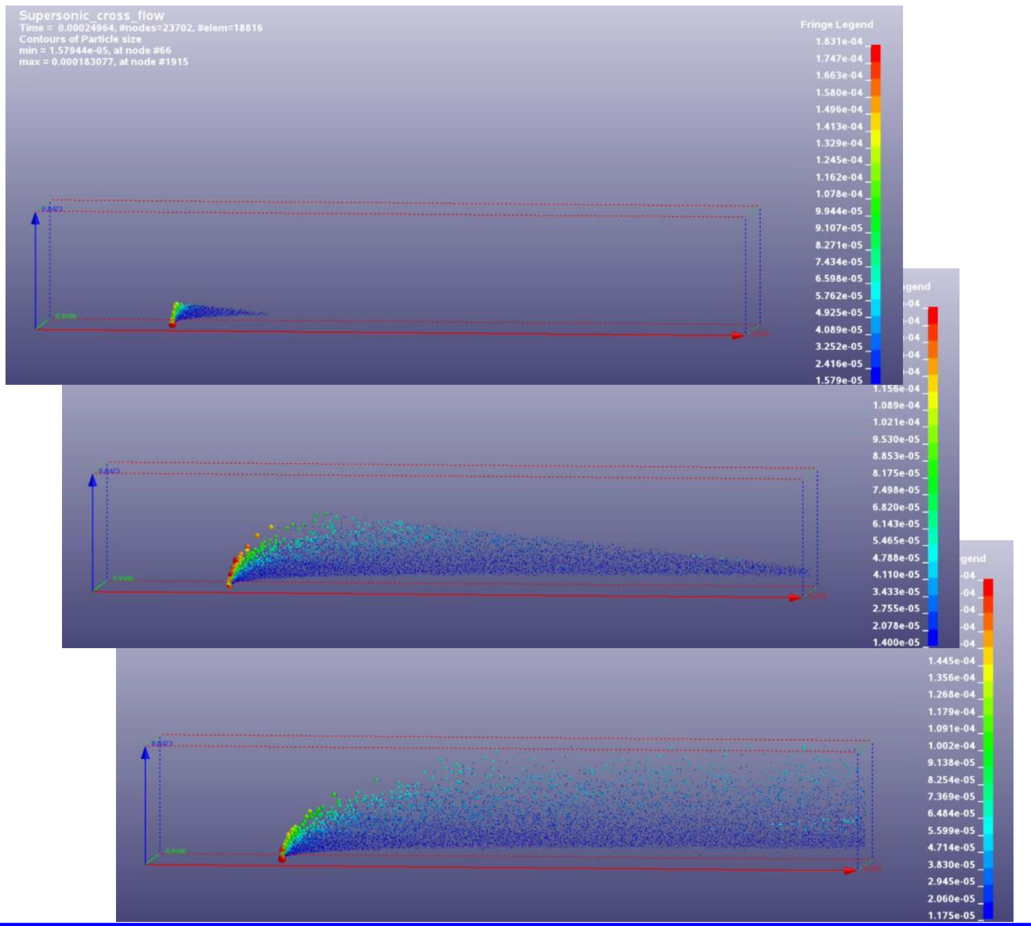
Pressure fringe of a ramped duct:
Hypersonic inflow at Ma = 4 & T = 500 K

Spray and particle dispersion:

Water spray jet



Supersonic cross flow



Solver features

2.1 Focus on the CESE scheme

2.2 Focus on the stabilization techniques

2.3 Focus on the chemistry coupling

2.4 Future developments

Reminder about the CESE method:

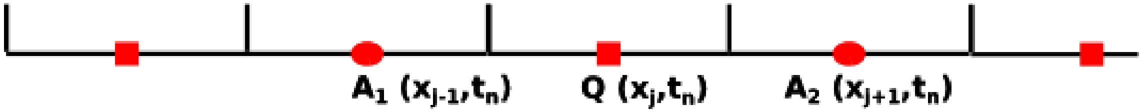
- CESE method : A novel CFD method for compressible flows
- CESE: **Conservation Element** & **Solution Element**
- 2nd order, explicit scheme
- Some important features of CESE method:
  - **Flux conservations** in **space-time** (locally & globally)
  - More accurate than normal 2nd order scheme
  - Flexible element shape
  - Simple but **very effective shock-capturing** strategy
  - Both strong shocks and small disturbances can be handled very well simultaneously

Two important concepts:

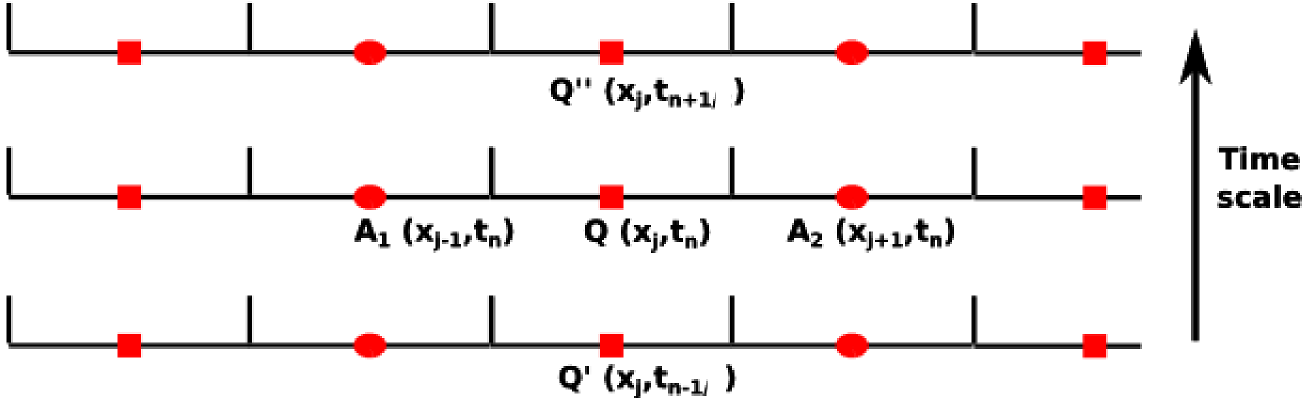
- **SE** — It is such a small region in the space-time domain around each grid point, in which the flow variables are assumed continuous and are approximated by some simple functions
- **CE** — It is a small region in the space-time domain, in which the conservation laws(integral equations) are enforced

Example of CESE 1D scheme:

- Step 1 **Element discretization**



- Step 2 **Expansion in the time dimension**
  (time acts as an additional spatial dimension)

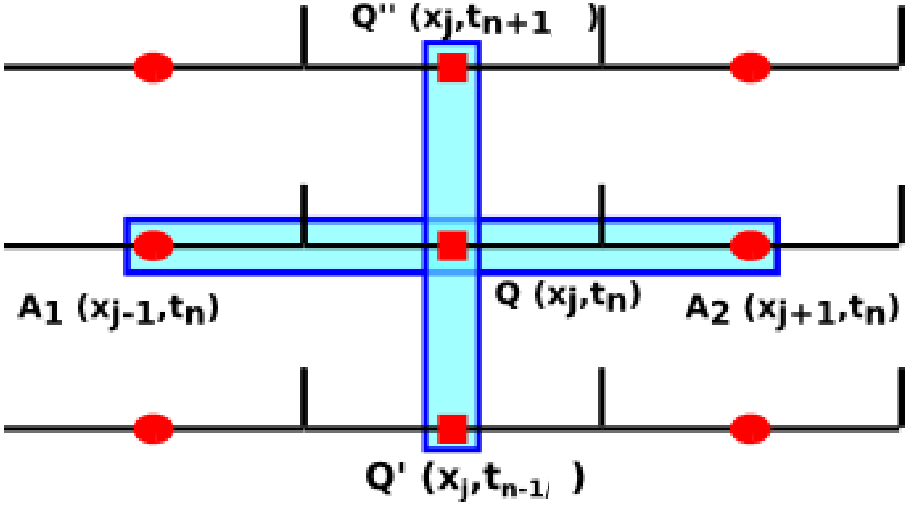


Example of CESE 1D scheme:

- Step 3 **Definition of a SE**

  - Along the SE domain, the flow variable will be approximated by a Taylor series

$$u^*(x,t) = u_q(x,t) + \frac{\partial u_q}{\partial x}(x - x_q) + \frac{\partial u_q}{\partial t}(t - t_q)$$



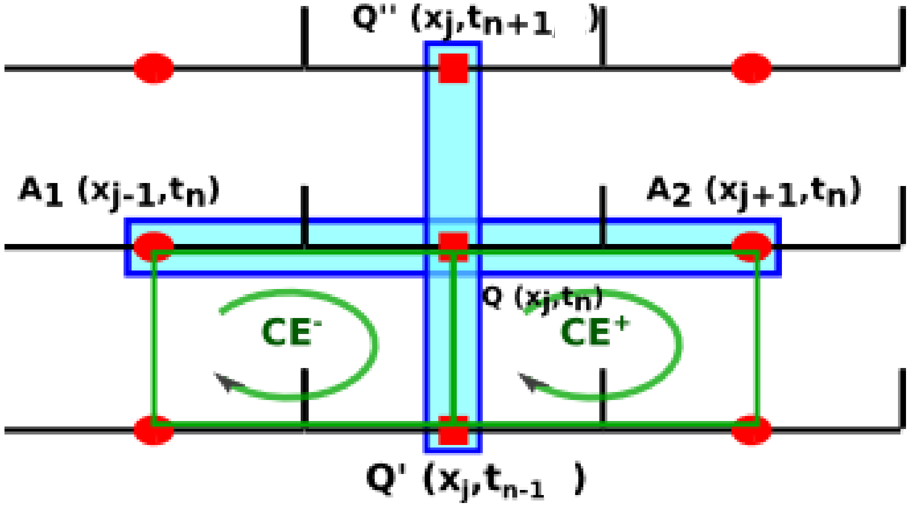
  - The time and spatial derivatives can be related by using the flow convection-diffusion equation (Euler for perfect flows, N-S otherwise) so that only $u_q(x,t)$ and its spatial derivative $\frac{\partial u_q}{\partial x}$ remain as unknowns to solve

Example of CESE 1D scheme:

- Step 4 **Definition of a CE**

  - The space-time integral equation for flow conservation along the lines formed by a CE gives

$$\oint_{S(CE^{\pm})} \vec{h}_m^{*} \cdot d\vec{s} = 0$$



  - CE- and CE+ each yield two equations for the two unknowns $u_q(x,t)$, $\frac{\partial u_q}{\partial x}$ function of quantities expressed between *j-1* and *j+1* and *n-1*
  - This allows to solve the complete system

Solver features

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2.4 Future Developments

- The above scheme is perfect for linear equations (invertible, neutral stable)
- For nonlinear equations, some numerical diffusions should be added, then we can get a modified scheme (a–ε scheme)
- For flows with discontinuities, especially with shocks, a re-weighting procedure (limiter) should be applied (**a–ε-α-β scheme**), which is the approach used by the CESE solver
- The procedures for deriving 2D and 3D schemes are similar as the above

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- For the chemistry solver, a chemistry input file detailing the species the chemical composition, the reaction mechanism, along with the corresponding initial and boundary conditions must be provided as input (**CHEMKIN file**)
- Currently, LS-DYNA has four different combustion modules including **isobaric, isochoric**, **1-step reaction**, and **multiple-species reaction mechanism**
- In the case of detonation problems, a **one-dimensional initiation** model is calculated to be followed by **two- or three-dimensional detonating** flow simulations
- The one-dimensional solution is automatically saved to a file which the user designates so that later on, one can use this file for several individual simulations
- For general chemical reacting flow problems, both **Euler** and **Navier-Stokes flows** can be used along with the CESE solver

Example of the LS-DYNA chemistry input file for an H_2-O_2 reaction mechanism

SAMPLE 1

```
ELEMENTS
N  O
END
SPECIES
O2 N2 O N NO
END
THERMO
END
REACTIONS   CAL/MOLE
O2+M=2O+M                       3.6E+18  -1.00  -118240.
  N/1.0/ NO/1.0/
  REV /3.00E+15  -0.50        0./
N2+M=2N+M                       1.90E+17 -0.50  -224557.
  O/1.0/ NO/1.0/ O2/1.0/
  REV /1.10E+16  -0.50        0./
NO+M=N+O+M                      3.90E+20 -1.50  -150035.
  N2/1.0/   O2/1.0/
  REV /1.00E+20  -1.50        0./
O+NO=N+O2                       3.20E+09  1.00   -39148.
  REV /1.30E+10   1.00    -7114./
O+N2=N+NO                       7.00E+13  0.00   -75514.
  REV /1.56E+13   0.00        0./
N+N2=N+N+N                     4.085E+22 -1.50  -224557.
  REV /2.27E+21  -1.50        0./
O2+O=2O+O                       9.00E+19 -1.00  -118240.
  REV /7.50E+16  -0.50        0./
O2+O2=2O+O2                     3.24E+19 -1.00  -118240.
  REV /2.70E+16  -0.50        0./
O2+N2=2O+N2                     7.20E+18 -1.00  -118240.
  REV /6.00E+15  -0.50        0./
N2+N2=2N+N2                     4.70E+17 -0.50  -224557.
  REV /2.72E+16  -0.50        0./
NO+M=N+O+M                    7.80E+20 -1.50  -150035.
   O/1.0/  N/1.0/ NO/1.0/
  REV /2.00E+20  -1.50        0./
END
```

- For the stochastic particles, The **stochastic processes** deal with systems which develop in time or space in accordance with **probability theories**
- Such processes have now been added to LS-DYNA to simulate a **water spray, aerosol**, and any **liquid particle flows** using random variables and probability density functions
- For the water spray, the existing basic breakup model and most advanced hybrid breakup model, **TAB, and KH&RT**, respectively are implemented with particle collision models
- Simulations combining multi-physics modules such as simulations of spray (or liquid injection), evaporation, and combustion simultaneously are currently under investigation

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Future developments

- 2D CESE with FSI capabilities
- Non-inertial reference frame for turbomachinery applications

Thank you for your attention!