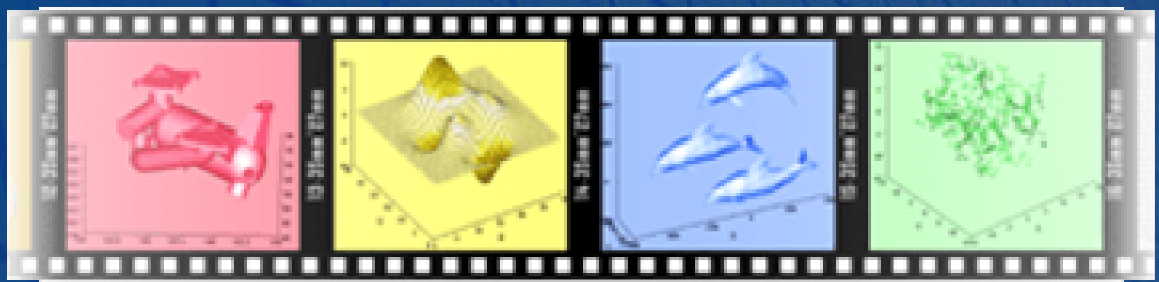
Visualizing the Physical Phenomena for Computational Science

with MATFOR® 4



Liger Chen
AnCAD **Inc.**

Outline

Introduction to **MATFOR®**

MATFOR® Functions

Cases Using **MATFOR®**

Visualization of Physical Problem by **MATFOR®**

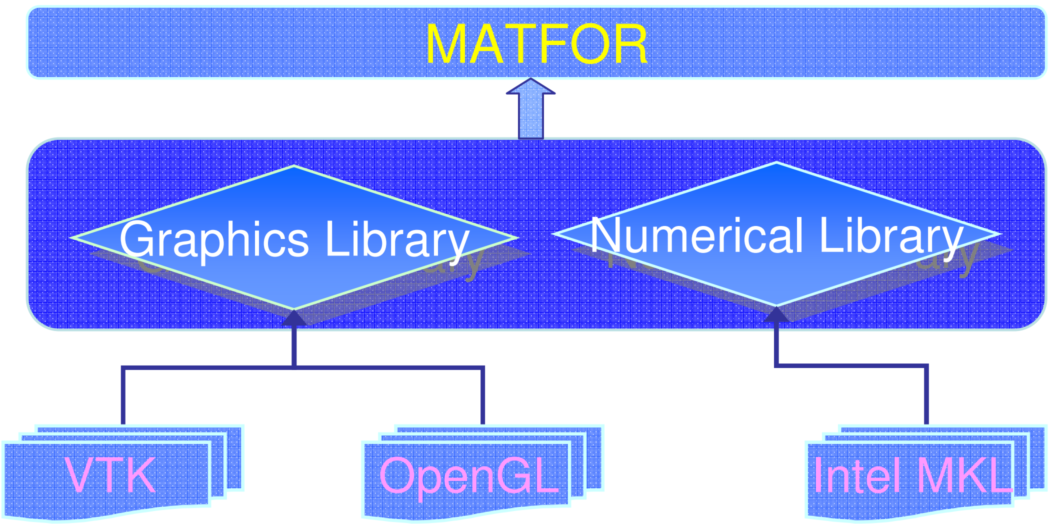
Introduction to MATFOR®

What's MATFOR® ?

- MATFOR® is a set of numerical and visualization libraries especially designed for programmers in scientific computing field.
- MATFOR® is a new generation graphics library fully exploiting the modules and the array features of Fortran 90/95 and C++ languages.
- MATFOR® is a collection of high-level graphical procedures developed with the mission of reducing time spent on the program development.

MATFOR® Structure

MATFOR®, a set of numerical and visualization libraries, is developed to enhance programming in C++ and Fortran environments. Especially designed for scientists and engineers, MATFOR® fulfills the needs of speed and advanced visualization capabilities simultaneously.



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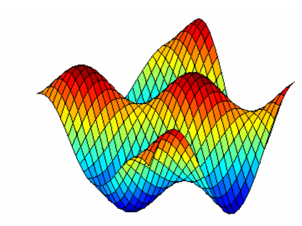
Numerical Library

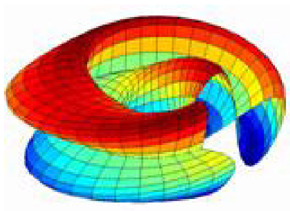
Based on Intel® MKL, the numerical library contains over 200 easy-to-use numerical functions subject to assist users with computational problem-solving.

- Data Manipulation Functions:
  mfSort, mfMin, mfMax, …
- Elementary Math Functions:
  mfSin, mfCos, mfASin, mfExp, mfAbs, …
- Elementary Matrix-Manipulating Functions:
  mfEye, mfDiag, mfRand, mfZeros, …
- Matrix Analysis:
  mfEig, mfInv, mfSvd, mfQz, mfLu, mfDet, mfNorm, …
- Sparse Array:
  msSpAdd, msSpSet, mfSpNNZ,mfSpLDiv,…
- File IO:
  mfSave, mfSaveAscii, mfLoad, mfLoadAscii, …

Graphics Library

Visualization Modules I


surf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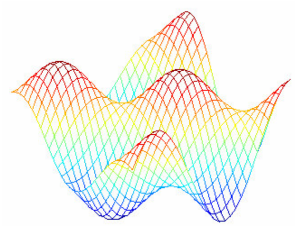
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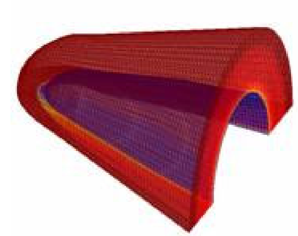
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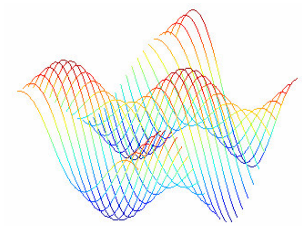
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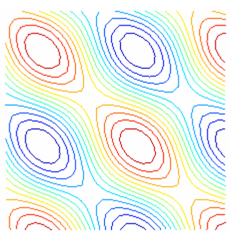
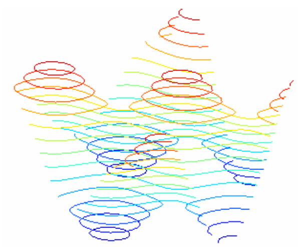

contour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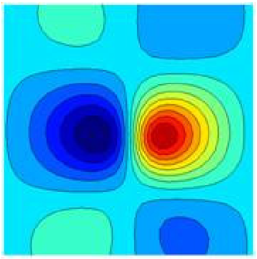
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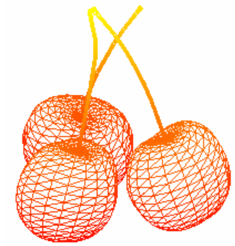
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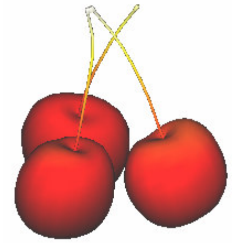
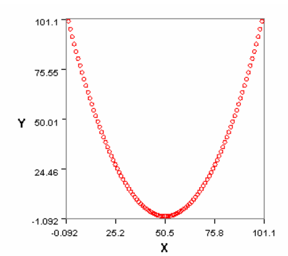
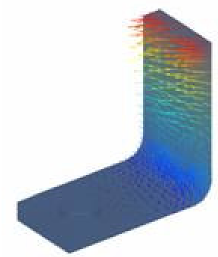

trisurf



plot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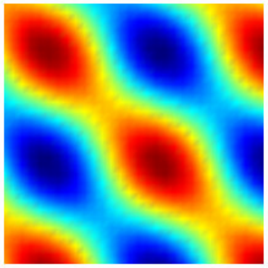
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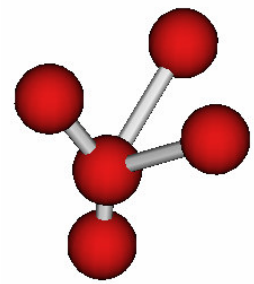
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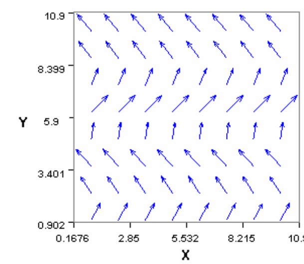
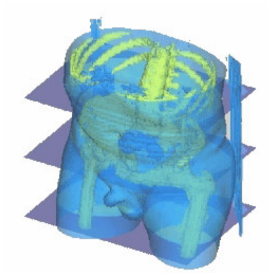
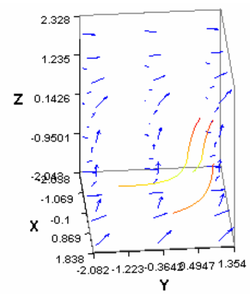


quiver

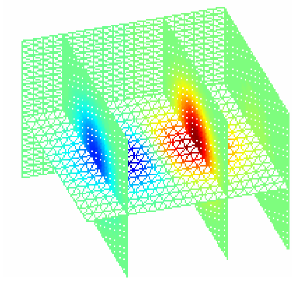
Graphics Library

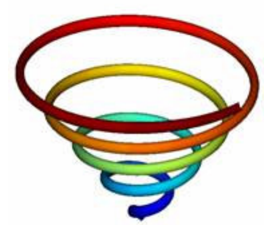
Visualization Modules II


isosurface



streamline


slices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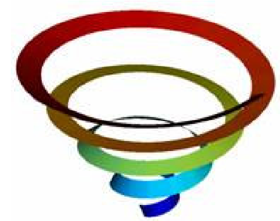
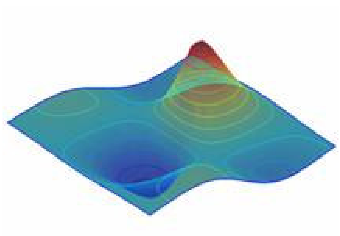

ribbon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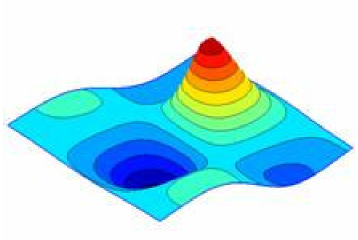
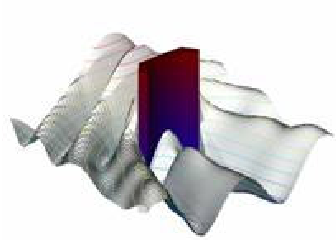
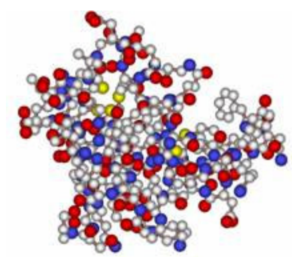
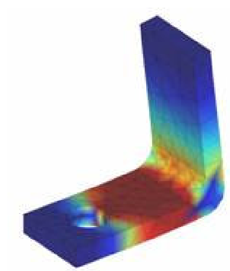
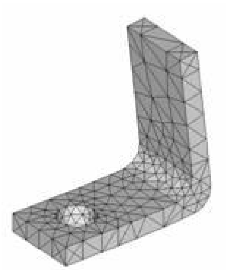

solidconour3

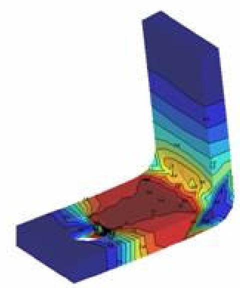

tricontour

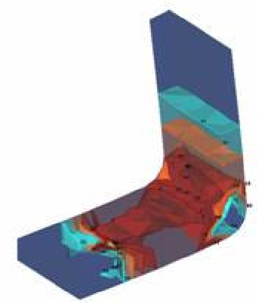

molecule

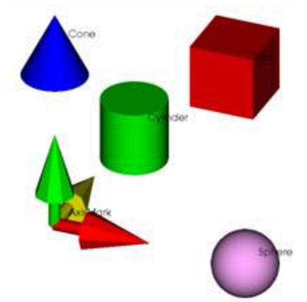

image


tetsurf


tetmesh


tetcontour

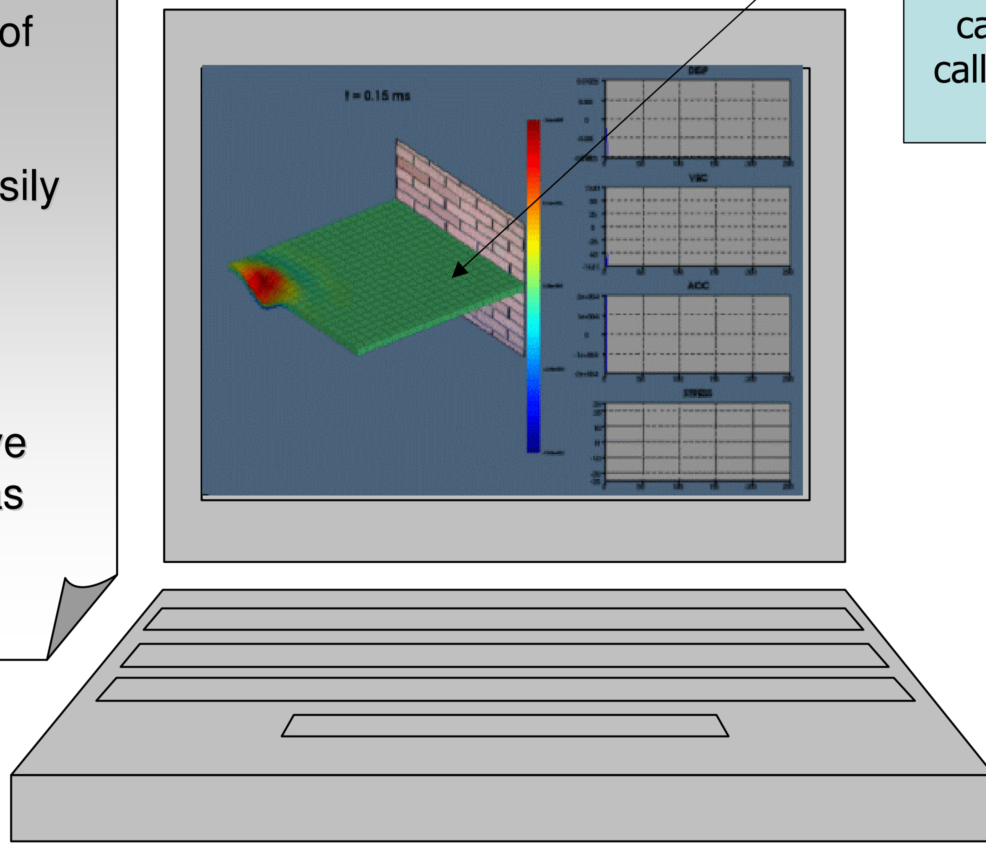

tetisosurface


cube, sphere, …

What Does MATFOR® Do?

By adding few lines of MATFOR® codes to your Fortran/C/C++ program, you can easily visualize your computing results, perform run-time animations, or even produce an interactive movie presentation as you execute your program.

```
…
call msSurf(x)
call msDrawNow
```

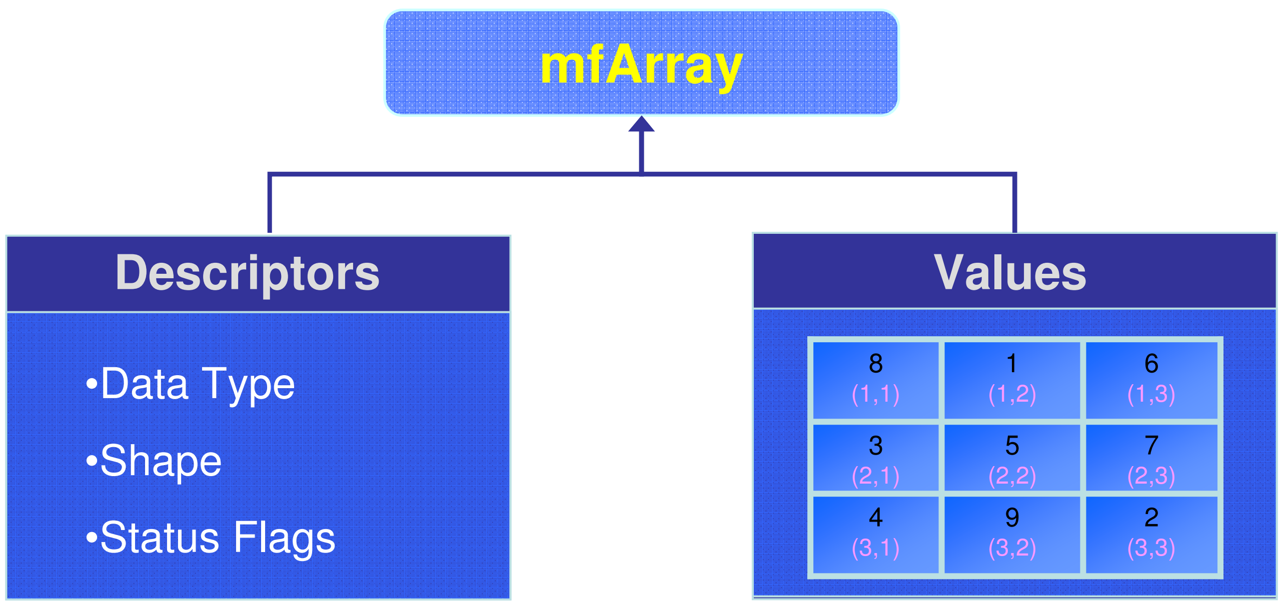


MATFOR® Functions

MATFOR® Dynamic Array I

mfArray Overview

mfArray is an advanced dynamic array defined by MATFOR® using modern features of C++ and Fortran 90/95. The mfArray data type consists of descriptors and values.



MATFOR® Dynamic Array II

mfArray Feature

A key to integrate MATFOR® toolkit into high-level programming environments

- Automatic data typing and dimensioning
- Dynamic memory allocation
- Simple calling routines with Matlab-like syntax

Construct and initialize the mfArray

C/C++	Fortran

mfArray x,y;
x = mfMagic(5);
y = mfInv(x);
	type(mfArray)::x,y
	x = mfMagic(5)
	y = mfInv(x)

Simple Using Mathmatical functions

- Besides its simple and powerful visual functions, MATFOR® enables scientists and engineers to code in Matlab fashion using the simple calling concept in Fortran and C++ environments.

MATLAB	a = inv(x)	e = eig(x)
MATFOR	a = mfInv(x)	e = mfEig(x)

- Calling msSVD in MATFOR® to perform singular value decomposition gives the same result as calling DGESVX in LAPACK. However, MATFOR® function only takes 3 pre-initialized parameters while LAPACK function takes 22 pre-initialized parameters.

```
Call DGESVX( FACT, TRANS, N, NRHS, A, LDA, AF, LDAF, IPIV, EQUED, R, C,
B, LDB, X, LDX, RCOND, FERR, BERR, WORK, IWORK, INFO )
```

LAPACK

```
Call msSVD( mfOut(A, B), C )
```

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$$a(x)\frac{d^2y}{dx^2}+b(x)\frac{dy}{dx}+(c(x)-\lambda_m)y=0$$

- Solving the symmetric tridiagonal matrix problem :

$$\begin{pmatrix} C_{1,1} & C_{1,2} & 0 & \cdots & 0 \\ C_{2,1} & C_{2,2} & C_{2,3} & 0 & \vdots \\ 0 & C_{3,2} & \ddots & \ddots & 0 \\ \vdots & 0 & \ddots & \ddots & C_{n-1,n} \\ 0 & \cdots & 0 & C_{n,n-1} & C_{n,n} \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_n \end{pmatrix}=\lambda\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_n \end{pmatrix}$$

$$C_{p+1,p}=C_{p,p+1}$$

(this eigsystem problem maybe be the reduction of a 2nd order differential equation

subroutine tridib(n,eps1,d,e,e2,lb,ub,m11,m,w,ind,ierr,rv4,rv5)
lamda= w

LAPACK

eps1, lb, ub , m11 , lb , ind , ierr , rv4 , and rv5 = ????

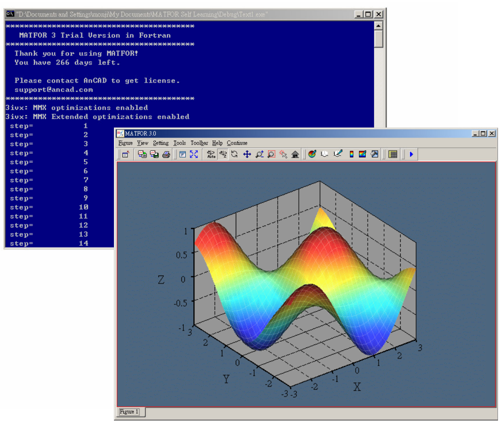
lamda = mfEig(x)

MATFOR

Real-Time Animation

MATFOR® features real-time program-monitoring mechanism to reduce time and effort spent on post-processing and debugging.

The simulation can be presented as an animation while the calculation is proceeded and shown in the console window.



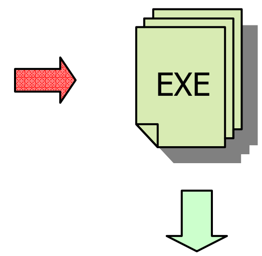
• MATFOR presenting simulation while calculating the data.

MATFOR® Sample Code

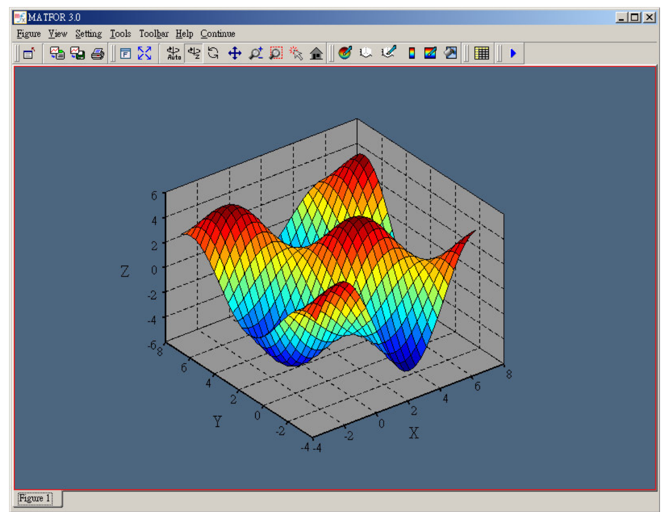
3D Presentation

```
program main

use fml
use fgl
! Declare mfArray variables
type(mfArray) :: x, y, z

! Construct grid matrices for 3D plot
call msMeshgrid(mfOut(x, y),
mfLinspace(-3,3,30), mfLinspace(-3,3,30))
! Calculate Z value
z = mfSin(x) * mfCos(y)
! Plot surf
call msSurf(x,y,z)
! Display the graph
call msViewPause
end program
```

demo codes



- MATFOR Standalone Executables



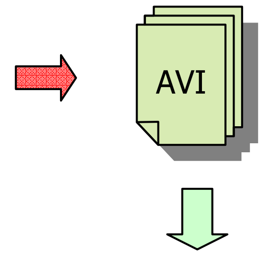
- MATFOR presents standalone executables.

MATFOR® Sample Code

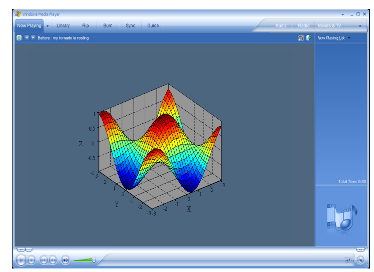
Movie Presentation

```
program main

use fml
use fgl

type(mfArray) :: x, y, z, h                     ! Declare mfArray variables
integer(4) :: I                                 ! Declare an integer variable
                                                ! Construct grid matrices for 3D plot
call msMeshgrid(mfOut(x, y), mfLinspace(-3,3,30), mfLinspace(-3,3,30))
call msRecordStart('demo.avi')                  ! Begin AVI recording
       do i=1,50                                ! Do loop
          write (*,*) 'step=', i
          z = mfSin(x+i/8.0d0) * mfCos(y)       ! Calculate Z value
          if (i==1) then                        ! Initialize handle
             h = mfSurf(x, y, z)
             call msDrawNow
          else
            call msGSet(h, 'zdata', z)          ! Update Z value
            call msDrawNow
          end if
       end do
call msRecordEnd                                ! End recording
call msViewPause                                ! Pause to display the graph

end program
```

demo codes



- Movie Files



- Viewing the recorded AVI file with media player.

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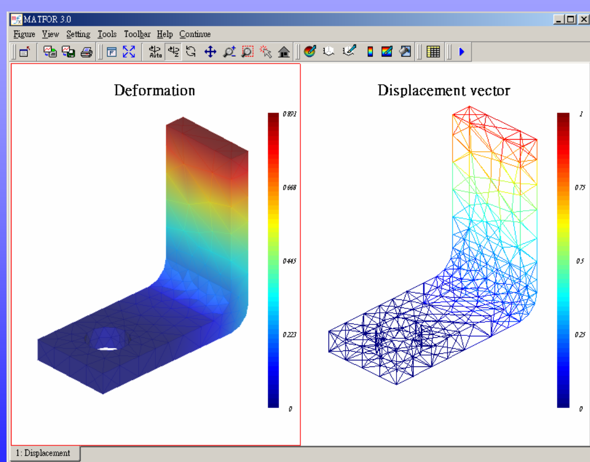
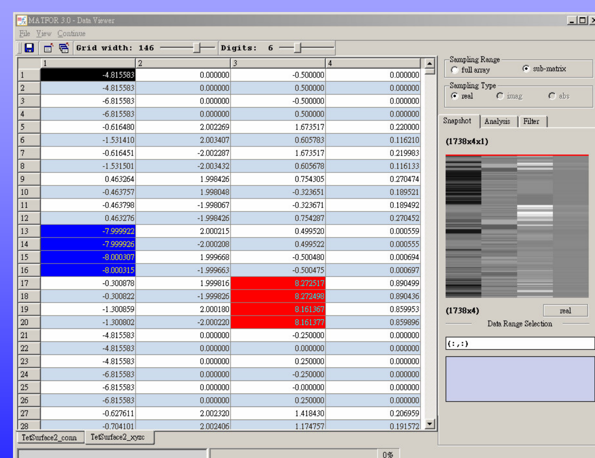
Runtime Data Manipulation

MATFOR® allows manipulation of the data displayed during execution; data can be examined with higher precision and customization at runtime.



- Graphics Viewer

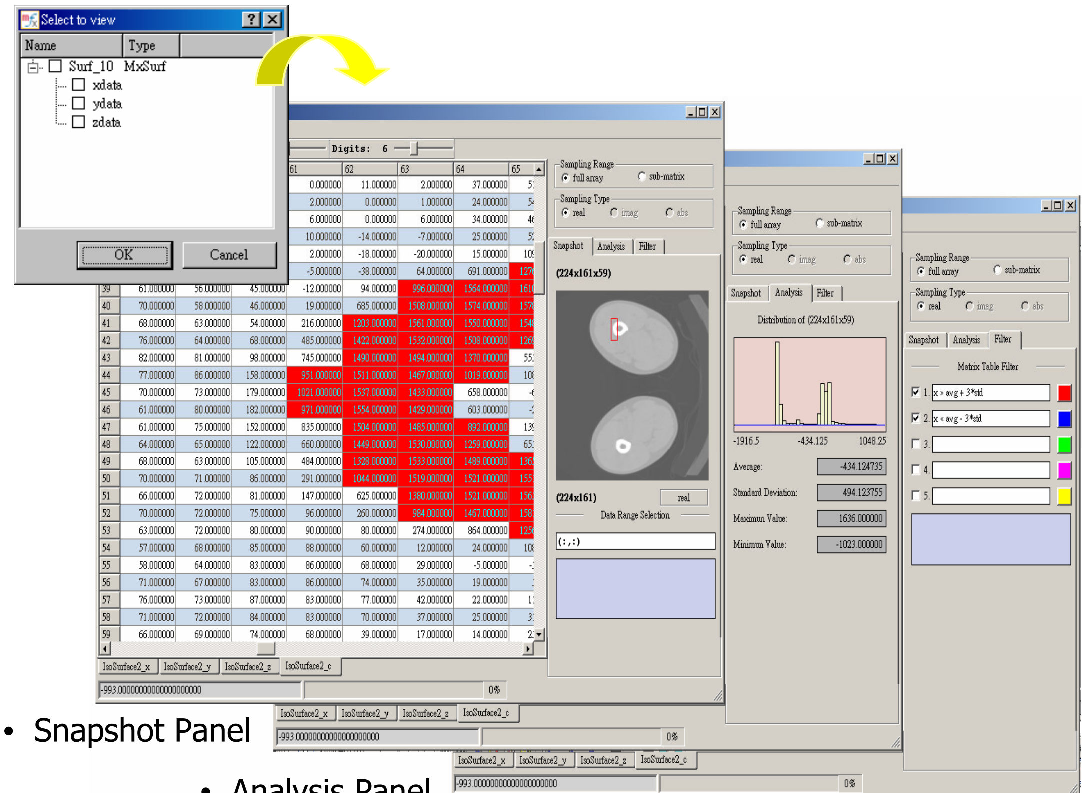


- Data Viewer

Data Viewer

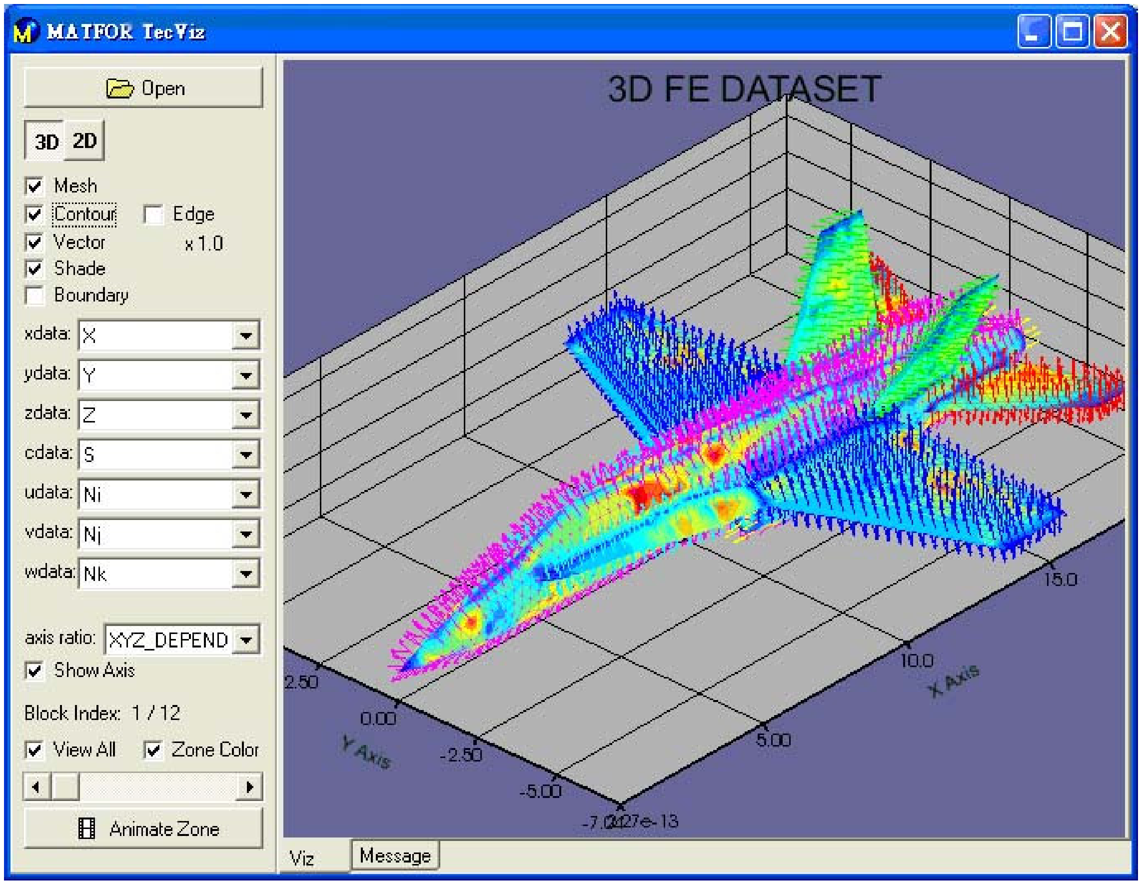
MATFOR® Data Viewer is a powerful tool that displays simulating data in a spreadsheet format.

- **Snapshot Panel**
  captures the snapshot of the distribution and size of the two dimensional data.
- **Analysis Panel**
  shows the distribution of the data including its average, standard deviation and min/max values.
- **Filter Panel**
  defines a range using conditions of inequalities.



- Snapshot Panel
- Analysis Panel
- Filter Panel

Supported Data File Formats

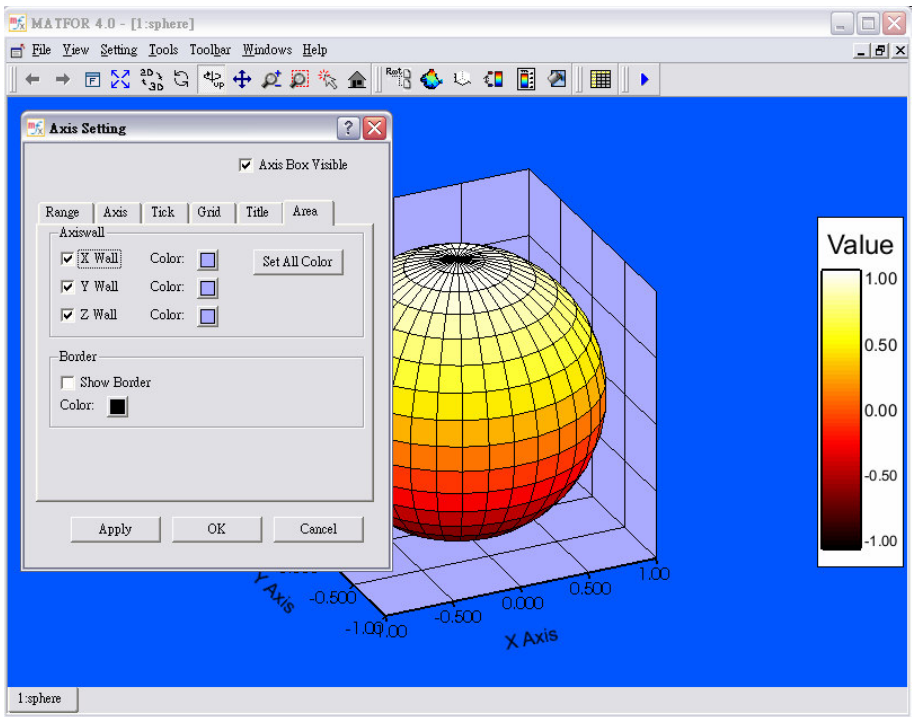


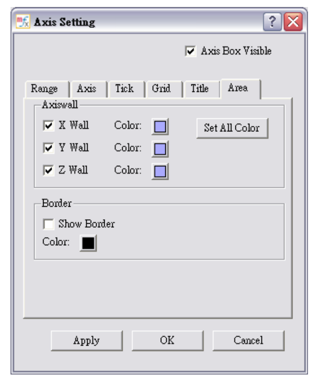
MATFOR 4 supports common software data formats and 3-D object formats to enhance the reusability and interchangeability of data.

- Matlab
- Tecplot
- 3DS, OBJ, and STL

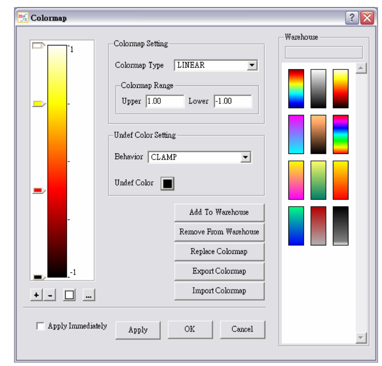
Graphics Viewer

MATFOR® Graphics Viewer provides a full range of graphical editing procedures which can be manipulated directly using the menu and the toolbar.

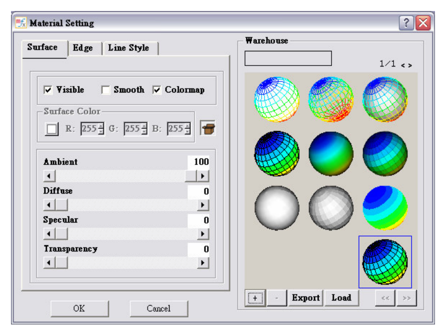




- Axis Setting Editor



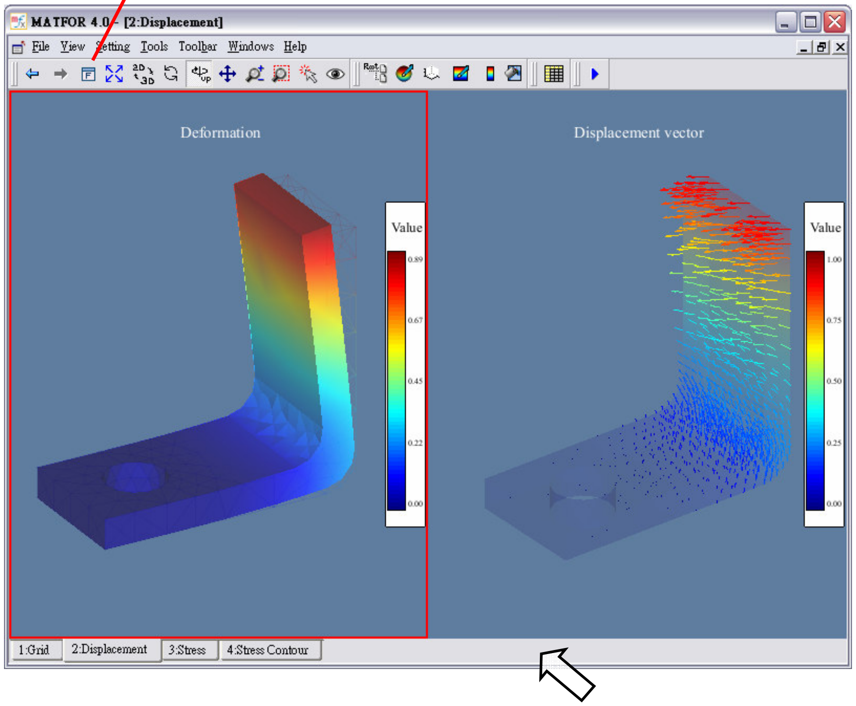
- Colormap Setting Editor



- Material Setting Editor

Enhanced Graphics Viewer
(Full-Screen Function)

Full Screen Mode



The full-screen function allows users to view and/or present data at full screen. This function also serves to eliminate the context for on-screen data capturing and printing.

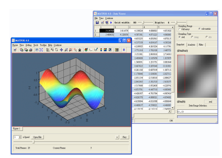
- Use the button indicated to show the graphs in full screen mode

MATFOR® mfPlayer

An exclusive Visual Tool

mfPlayer is an exclusive visual tool by which the previously saved numerical data is read and displayed as an interactive movie presentation. As MATFOR® saves the simulated data into a MATFOR®-defined MFA file, **mfPlayer** is one approach to present the recorded animation. The complete video clip can then be viewed from different angles.

- resize
- rotate
- zoom
- pause
- forward
- reward
- view data
- change colormaps

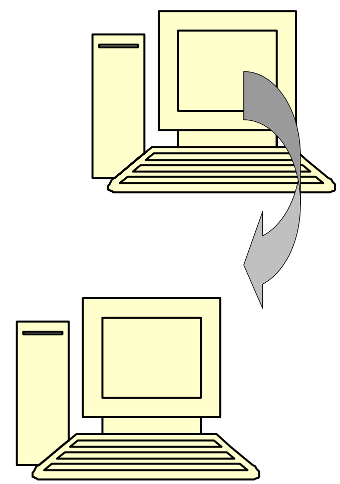


- Data Viewer
- mfPlayer

mfPlayer Standalone

- Currently, the proprietary format dominates in most visualization tools generates files that can only be executed on one specific application.
- MATFOR® possesses the ability to convert visualization files into standalone executables.
- Through the conversion, data sharing and publishing become much easier.

Compiling and linking the programs with MATFOR library.



Running compiled executables without installing MATFOR.

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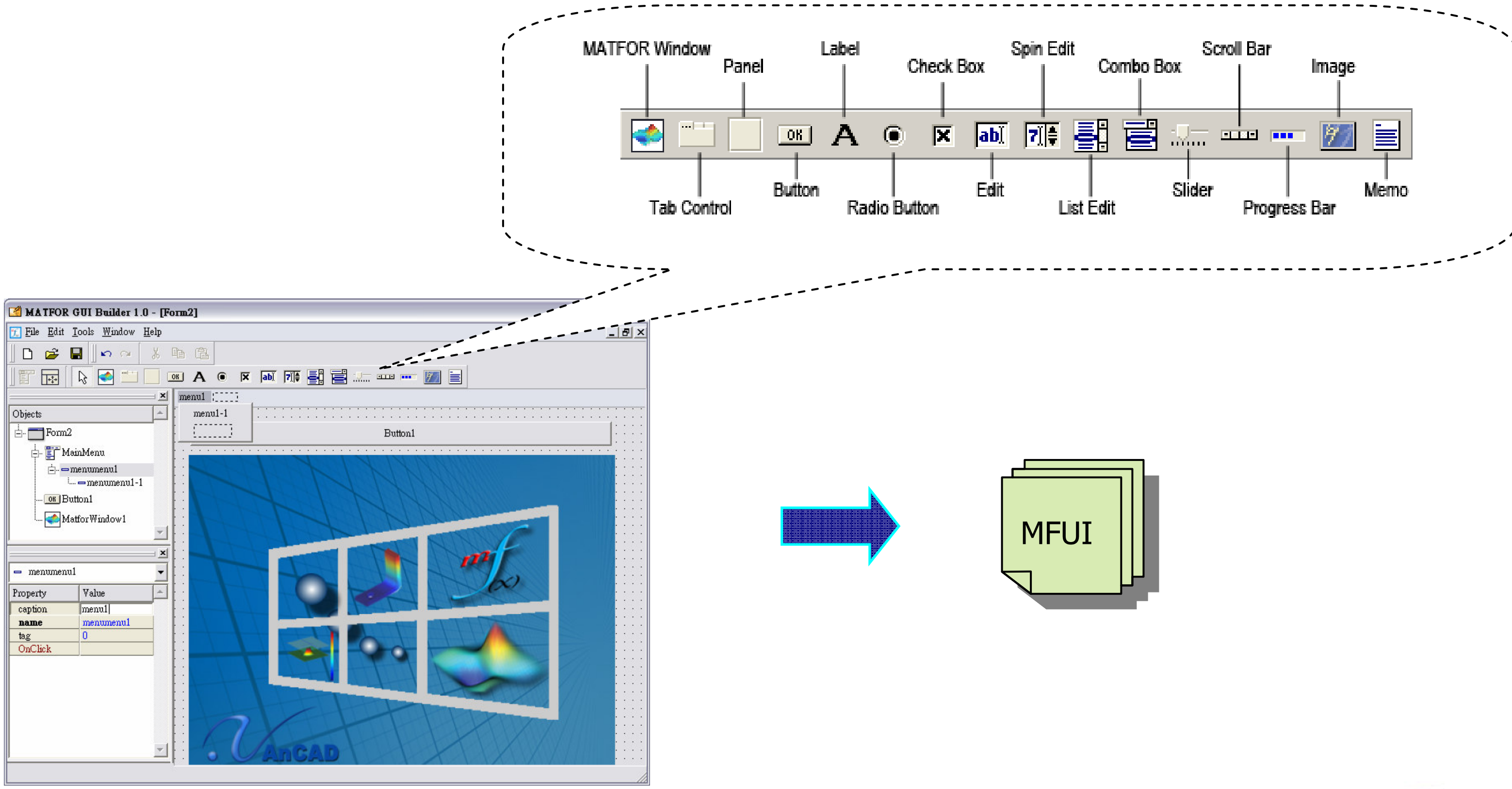
MATFOR® GUI Builder

MATFOR® GUI Builder allows users to customize an interface of their own; the interface can be saved into a MFUI file (based on XML format).

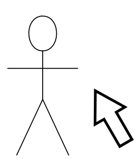


- MATFOR GUI Builder

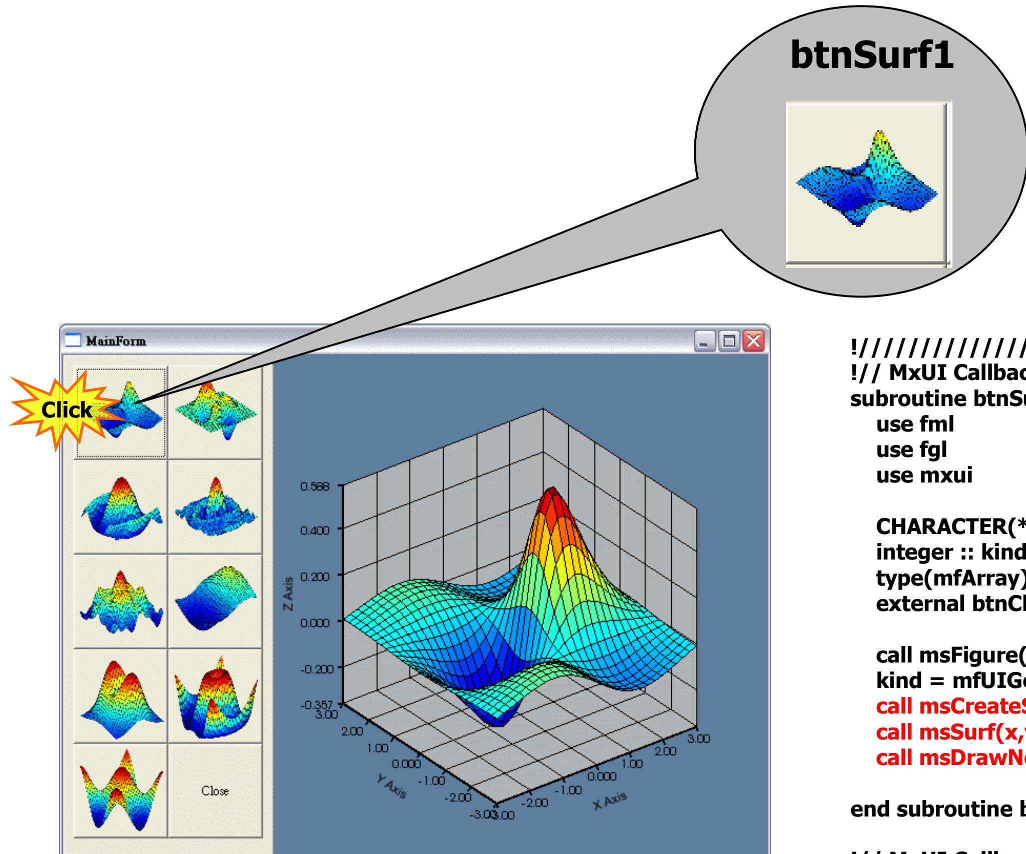
MATFOR® GUI System

(An Use Case)

- How does the communication work between the user and the application?

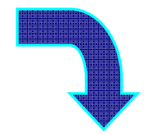


Actor



Application

UI Engine

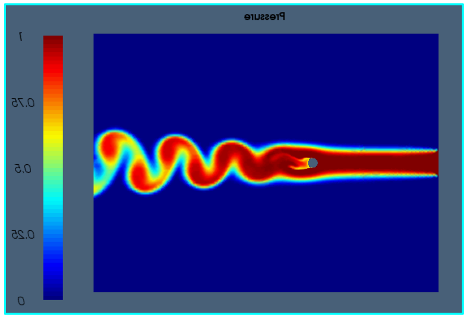


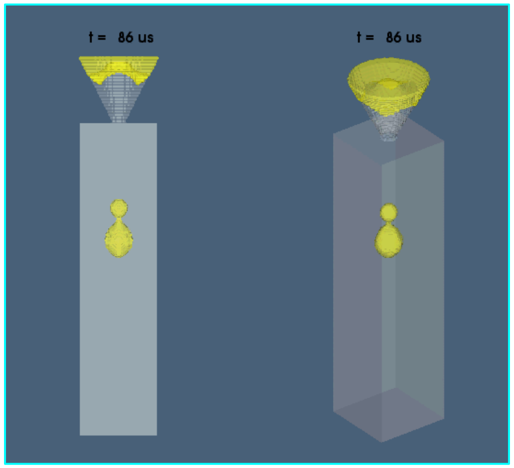
```
!//////////////////////////////////////////////////////////////////
!// MxUI Callback BEGIN
subroutine btnSurf_Click(sender)
   use fml
   use fgl
   use mxui

   CHARACTER(*) :: sender
   integer :: kind
   type(mfArray) :: x, y, z
   external btnClose_Click

   call msFigure()
   kind = mfUIGetPropertyInteger( sender, 'tag' )
   call msCreateSurfData( mfOut(x,y,z), mf(kind), mf(30), mf(30) )
   call msSurf(x,y,z)
   call msDrawNow

end subroutine btnSurf_Click

!// MxUI Callback END
!//////////////////////////////////////////////////////////////////
```

Cases Using MATFOR®

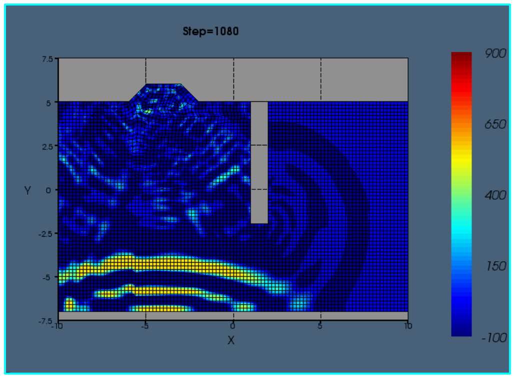
Applied Fields

- Solid Mechanics
- Fluid Dynamics
- Astrodynamics

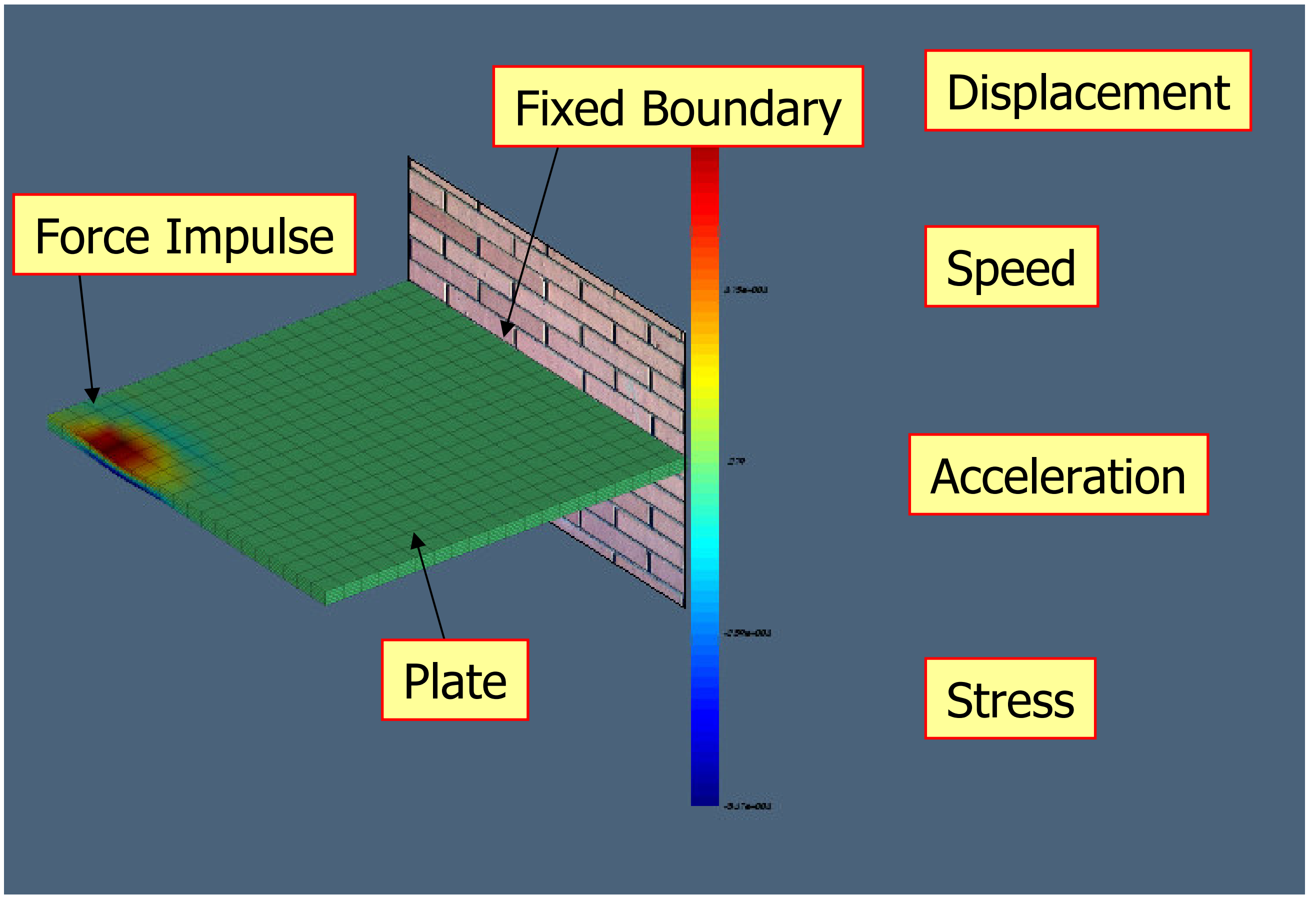




- Electromagnetic Analysis
- Heat Transfer and Geology Analysis
- Optical propagation
- Molecular Dynamics



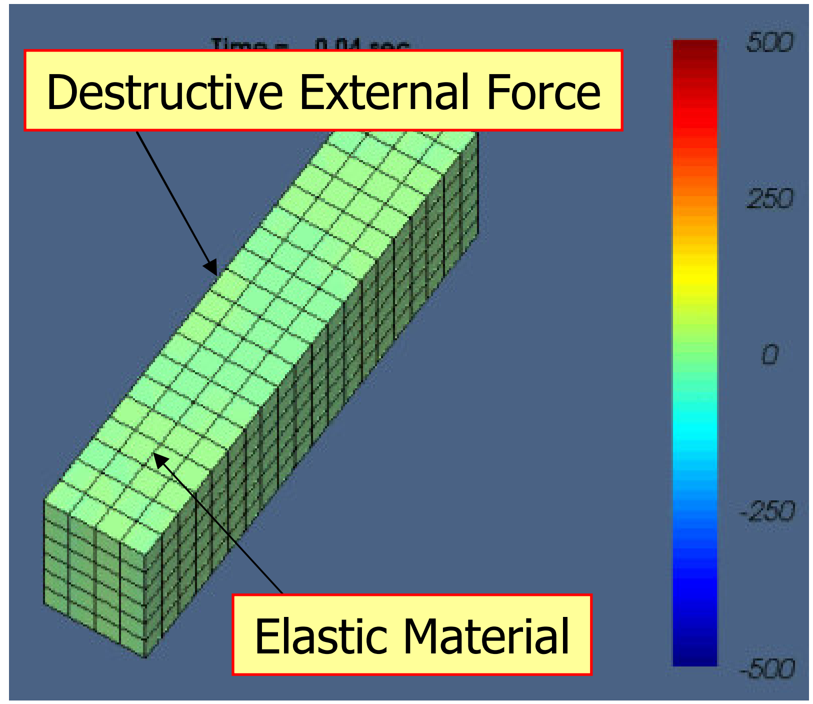
Thin-plate Vibration Analysis



(Data courtesy of Yuan-Sen Yang, National Center for Research on Earthquake Engineering)

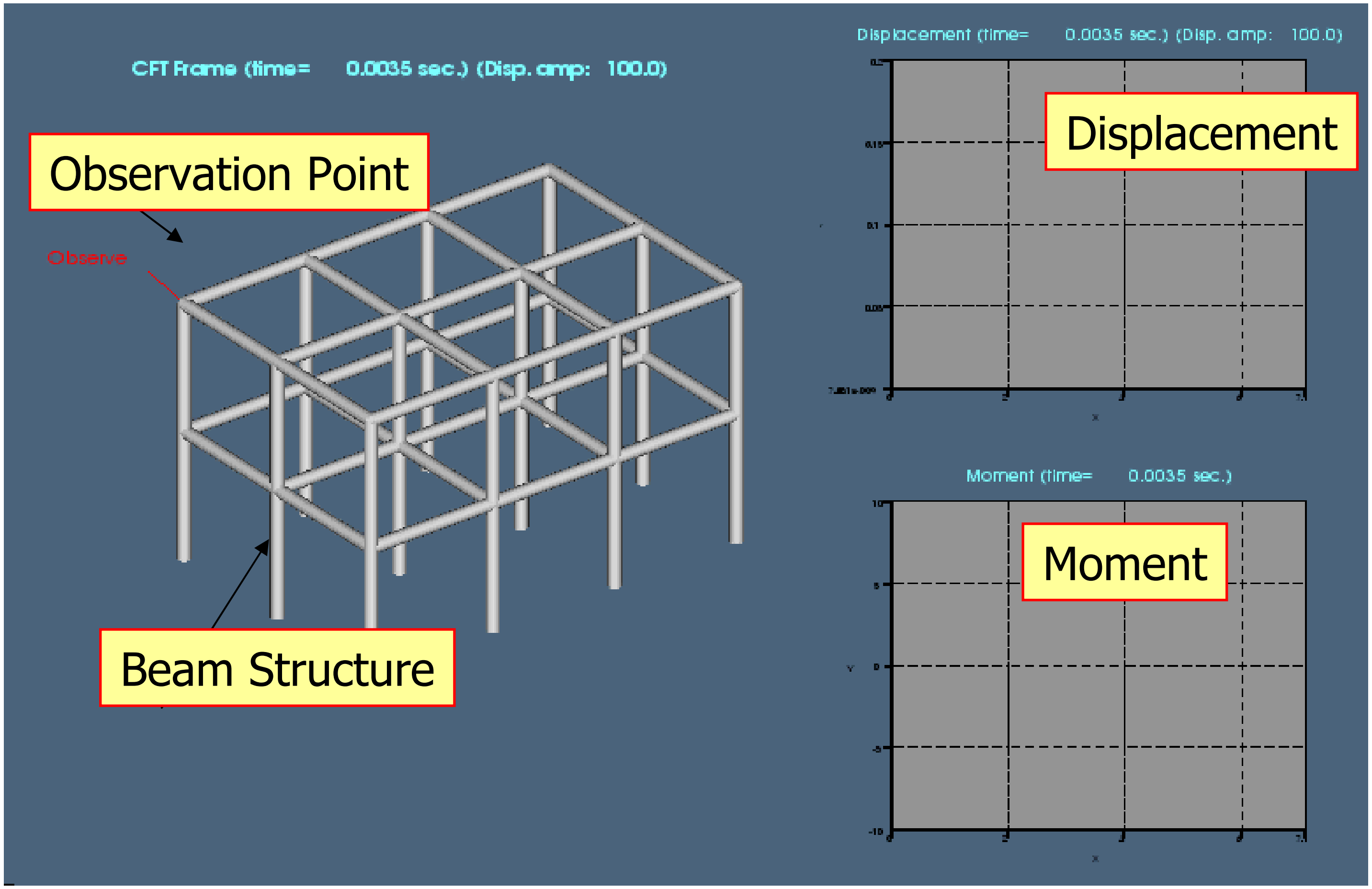
3D Co-rotational Explicit Finite Element Analysis

Simulation of the nonlinear, nonconsecutive destructive phenomenon of the dam structure based on the finite element method.



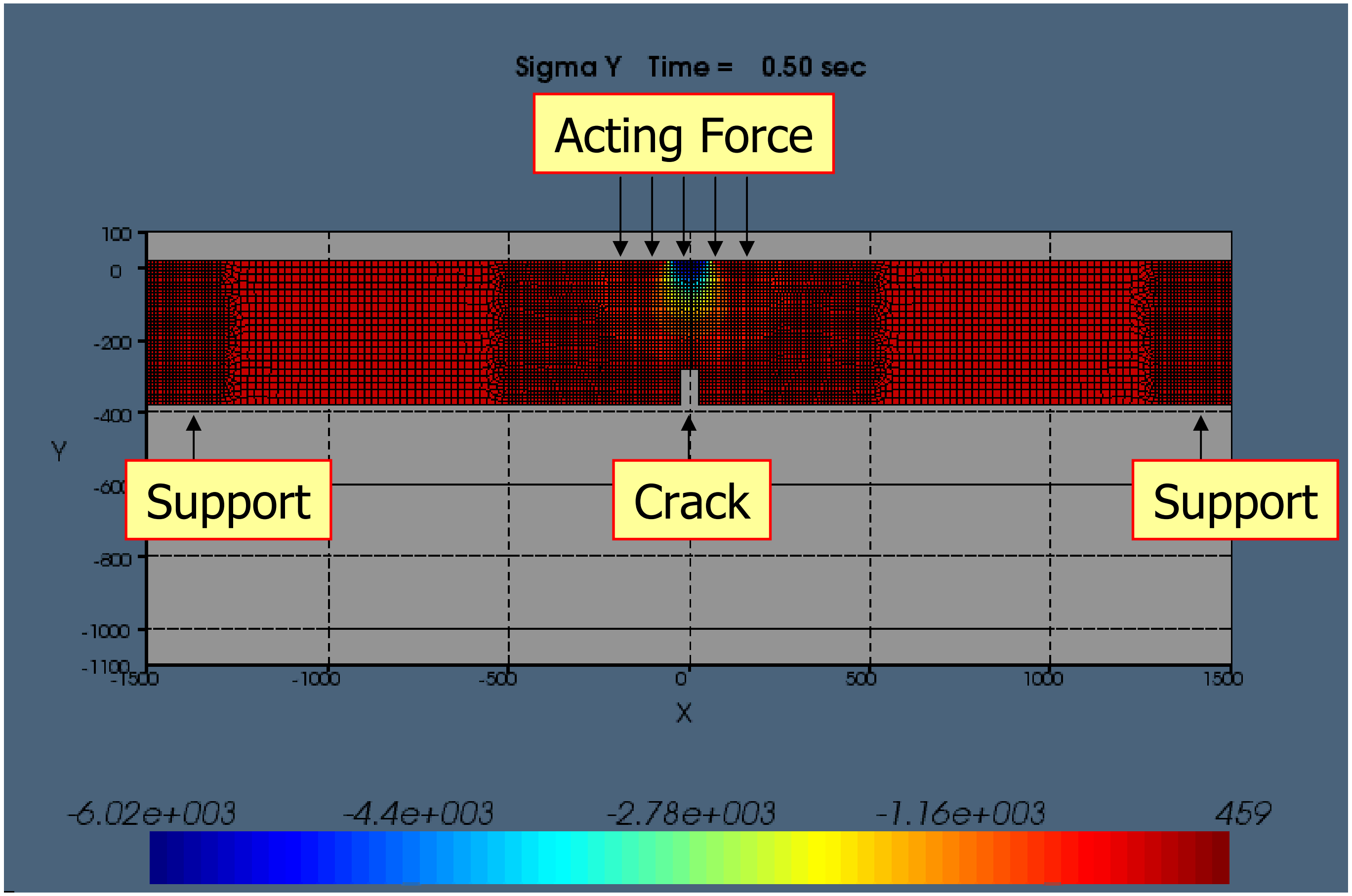
(Data courtesy of Professor Edward C. Ting/Chih-Cheng Lin, National Central University)

Structural Earthquake Response



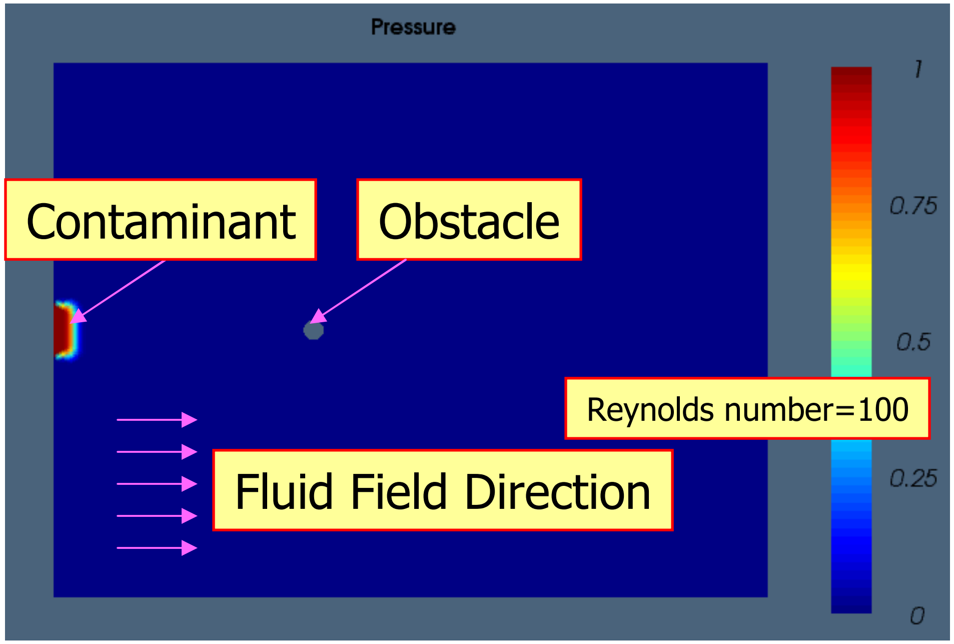
(Data courtesy of Professor Yuan-Sen Yang, National Center for Research on Earthquake Engineering)

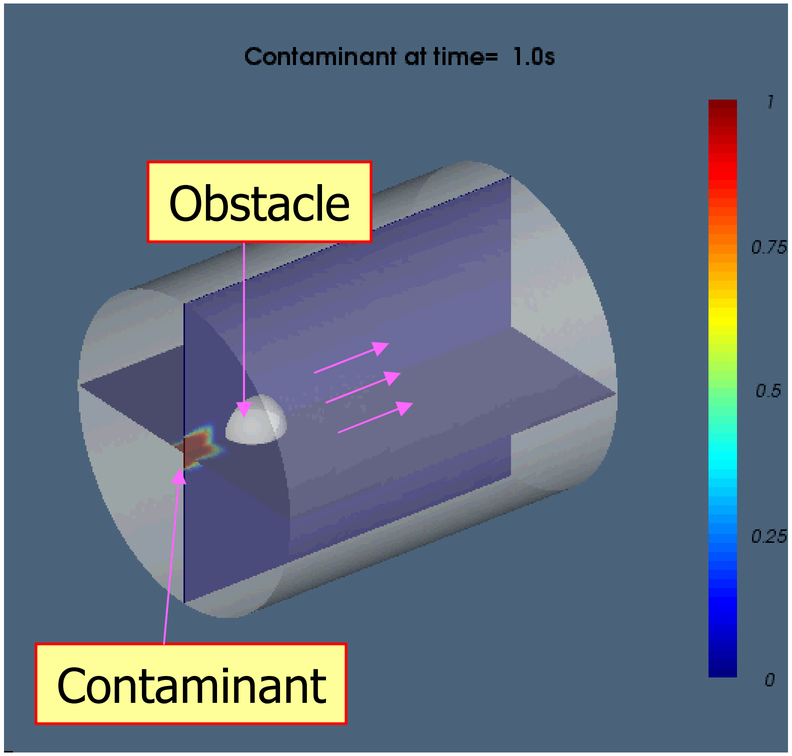
Concrete Fracture 2D Analysis



(Data courtesy of Professor Edward C. Ting/Yeh-Chan Lin/Chih-Cheng Lin, National Central University)

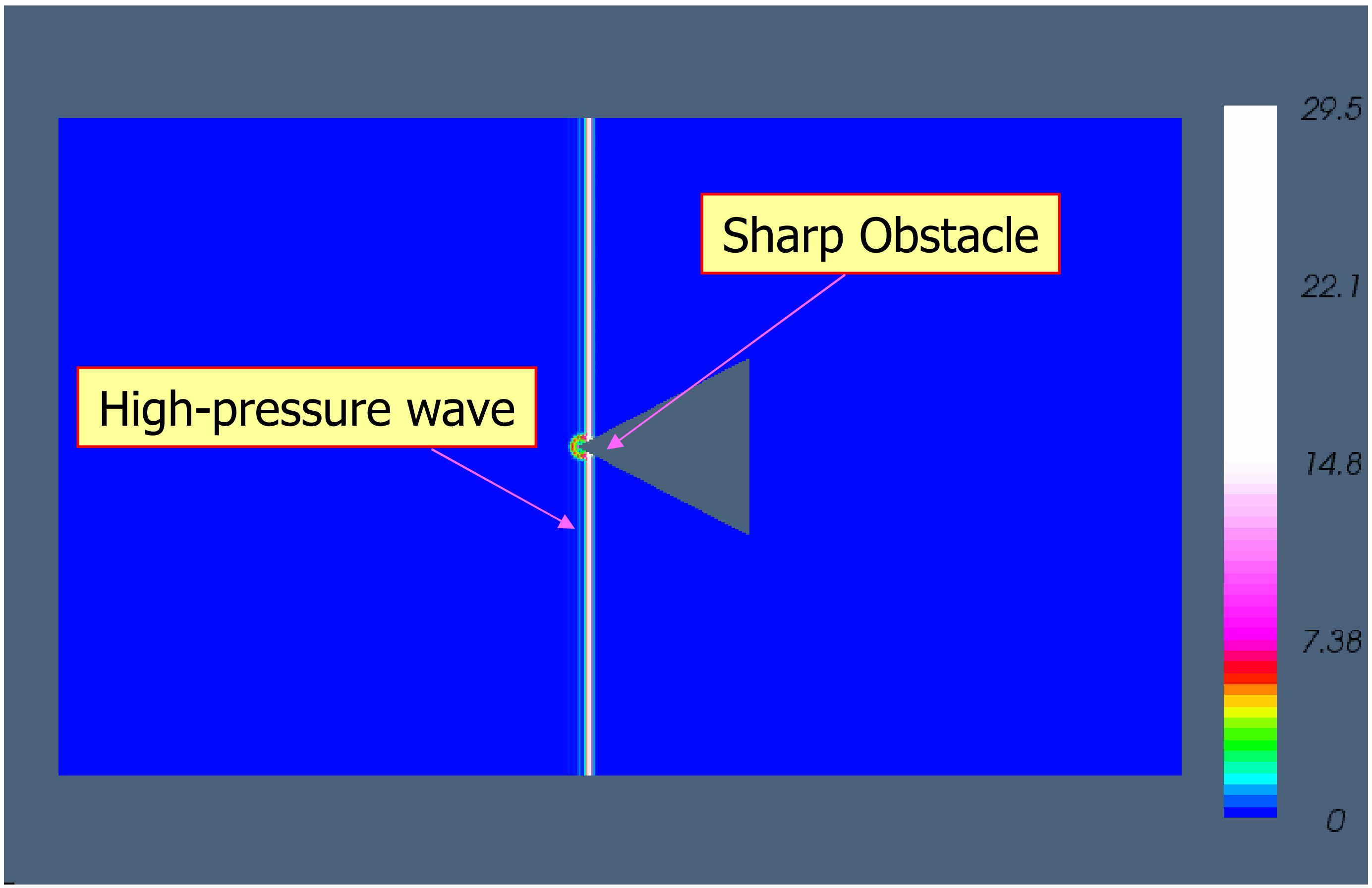
Fluid Field Turbulence I





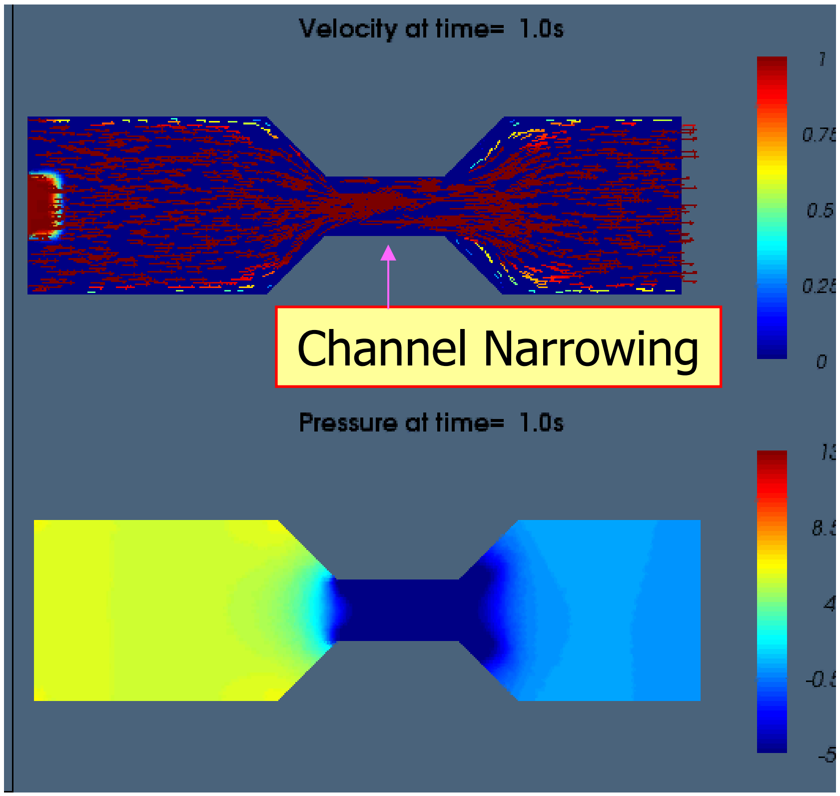
(Data courtesy of Ming-Hsin Su, AnCAD, Inc.)

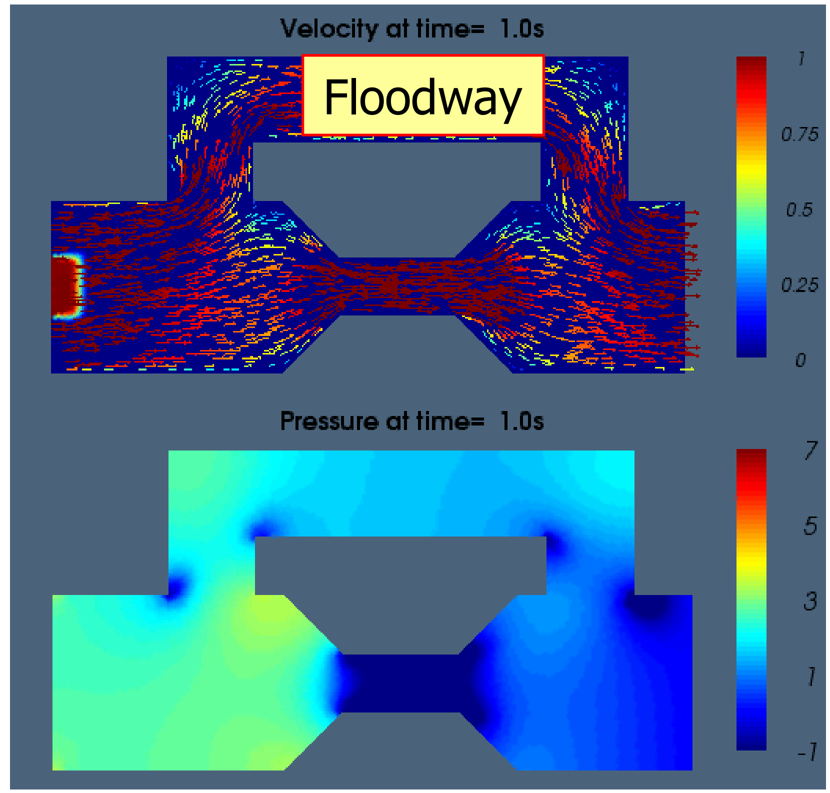
High Pressure Reflection



(Data courtesy of Dr. Lin and Dr. Huang, Institute of Science and Technology)

Fluid Field Turbulence II

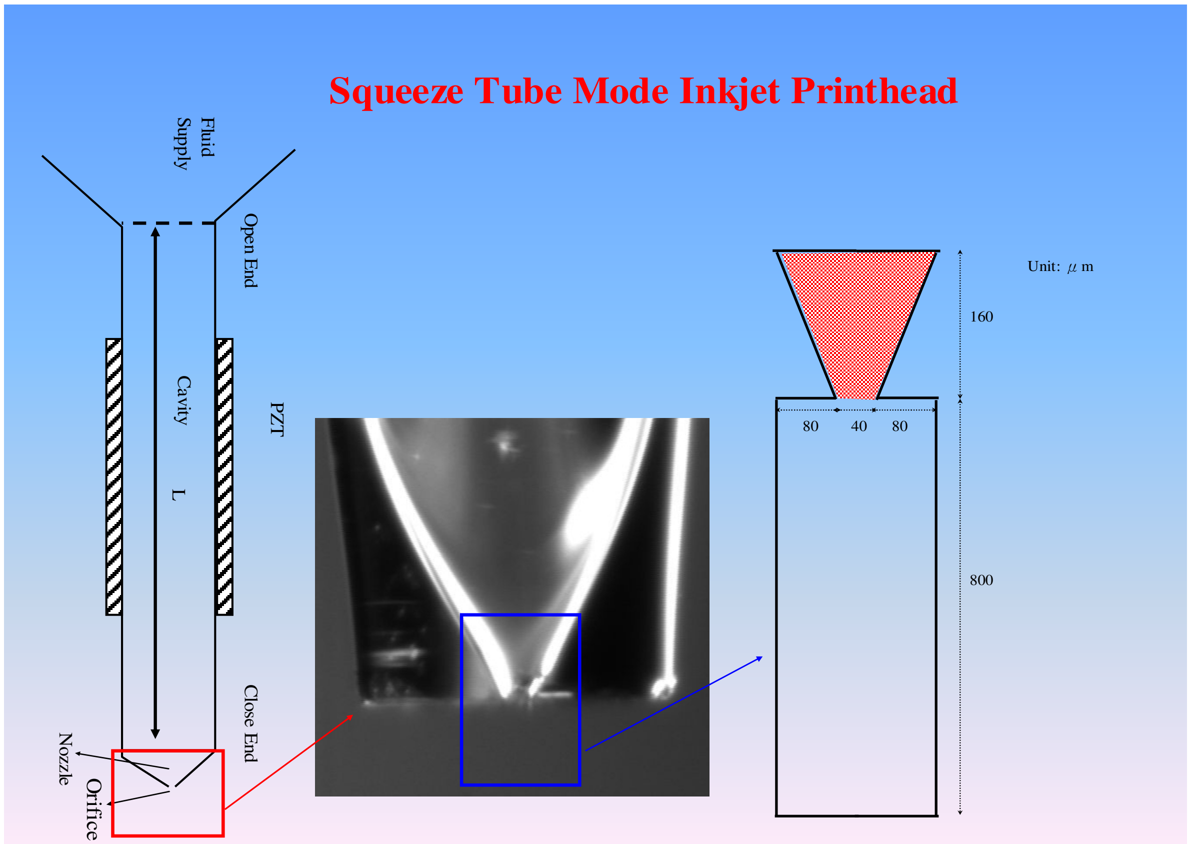




(Data courtesy of Ming-Hsin Su, AnCAD, Inc.)

3D Inkjet System Simulation I

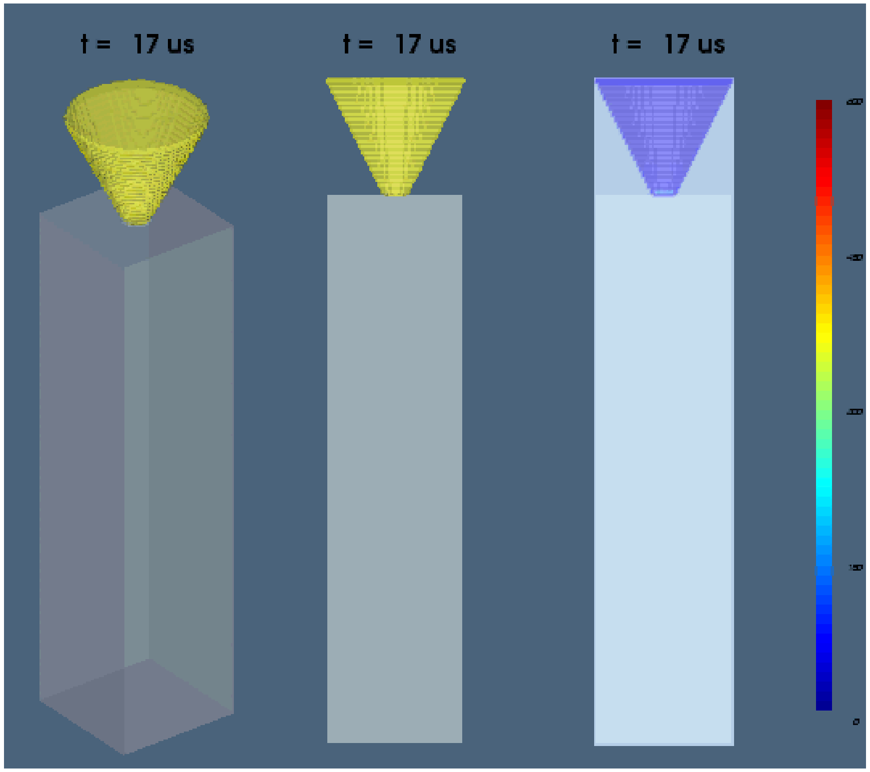
Blue Print

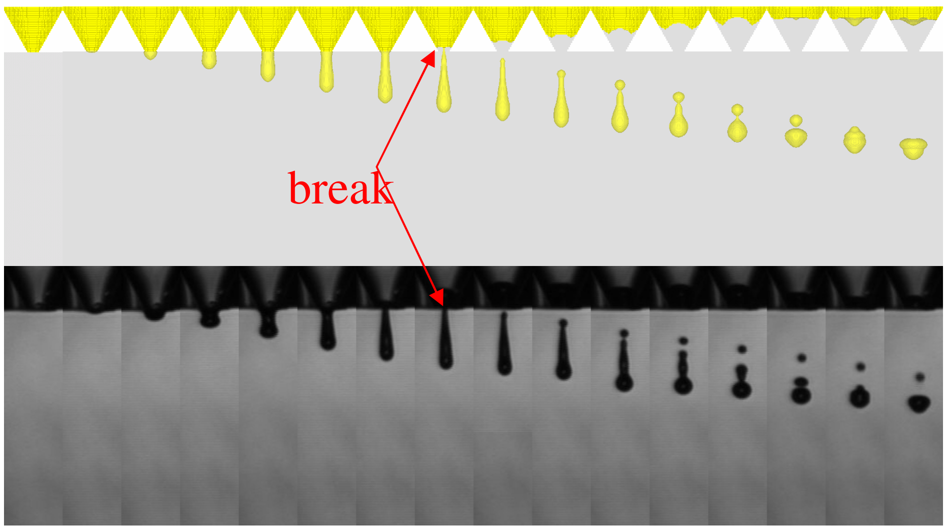


(Data courtesy of Weng-Sing Huang/Hsuan-Chung Wu, National Cheng Kung University)

3D Inkjet System Simulation II

Computer Simulation

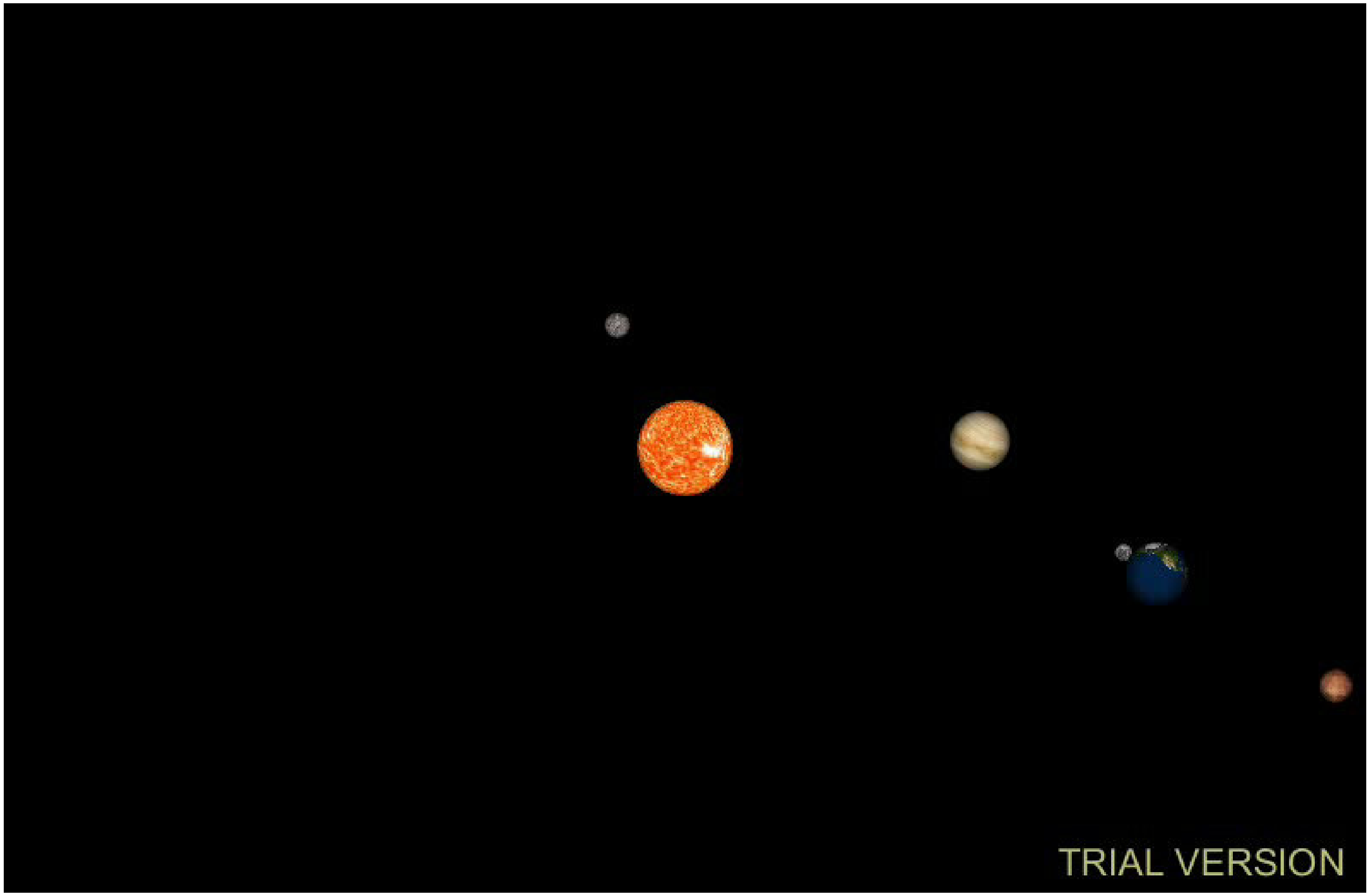




Time: 0 20 26 32 38 44 50 56 62 68 74 80 [μ s]

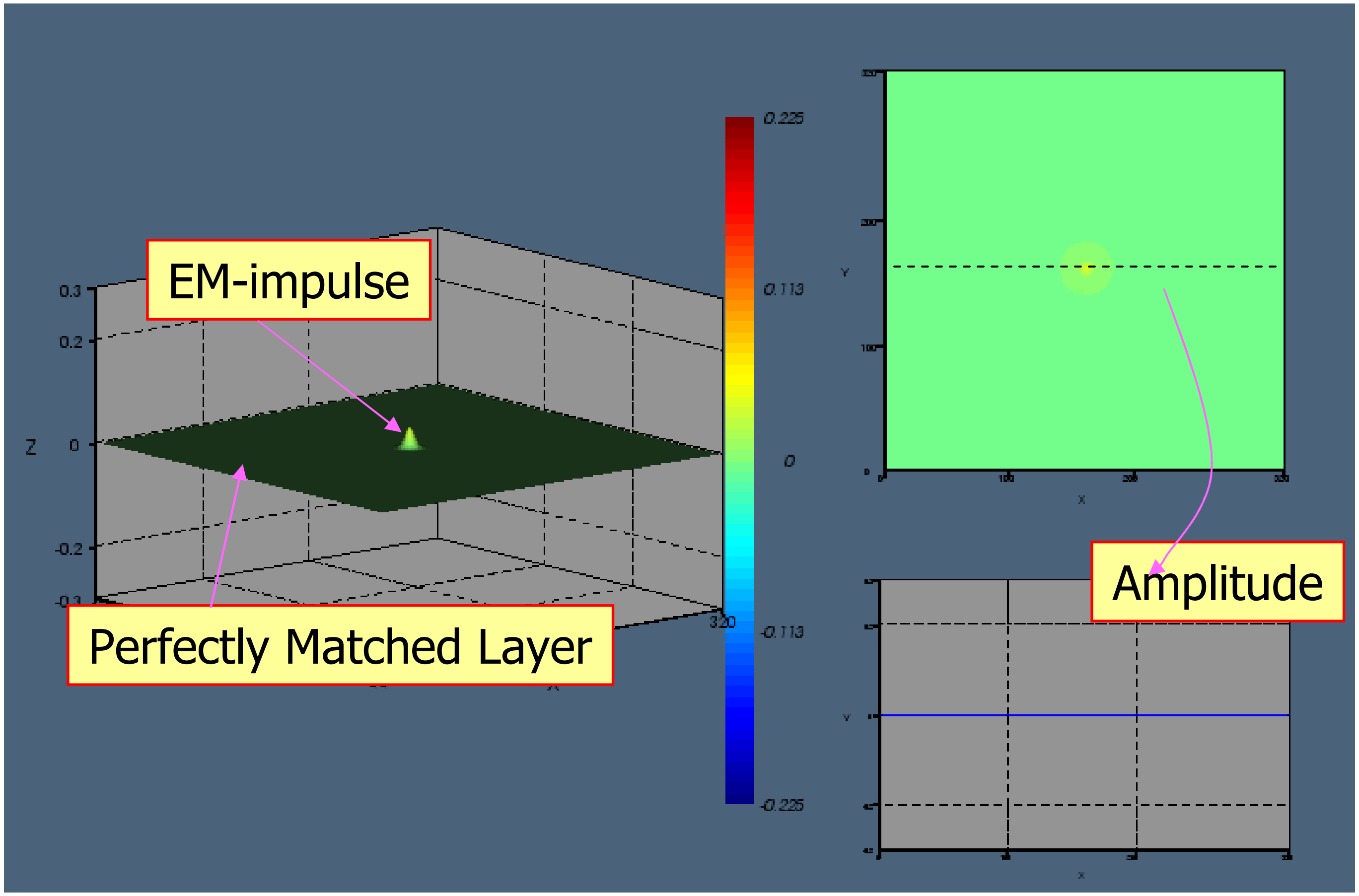
(Data courtesy of Weng-Sing Huang/Hsuan-Chung Wu, National Cheng Kung University)

3D Solar System Model



(Data courtesy of Li-Ger Chen, AnCAD, Inc.)

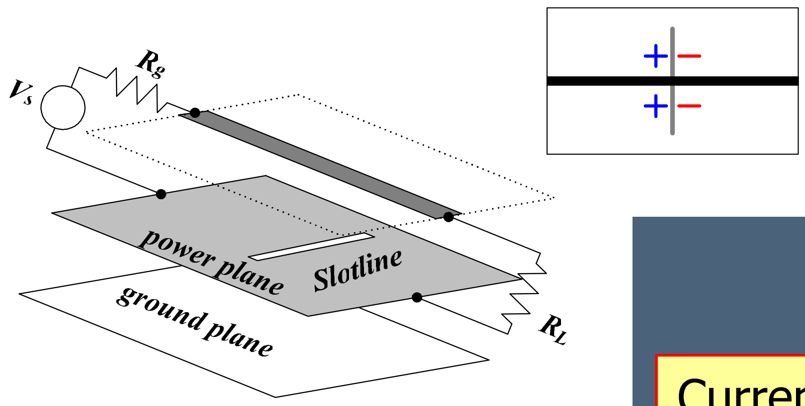
EM-wave Scattering on Perfectly Matched Layer

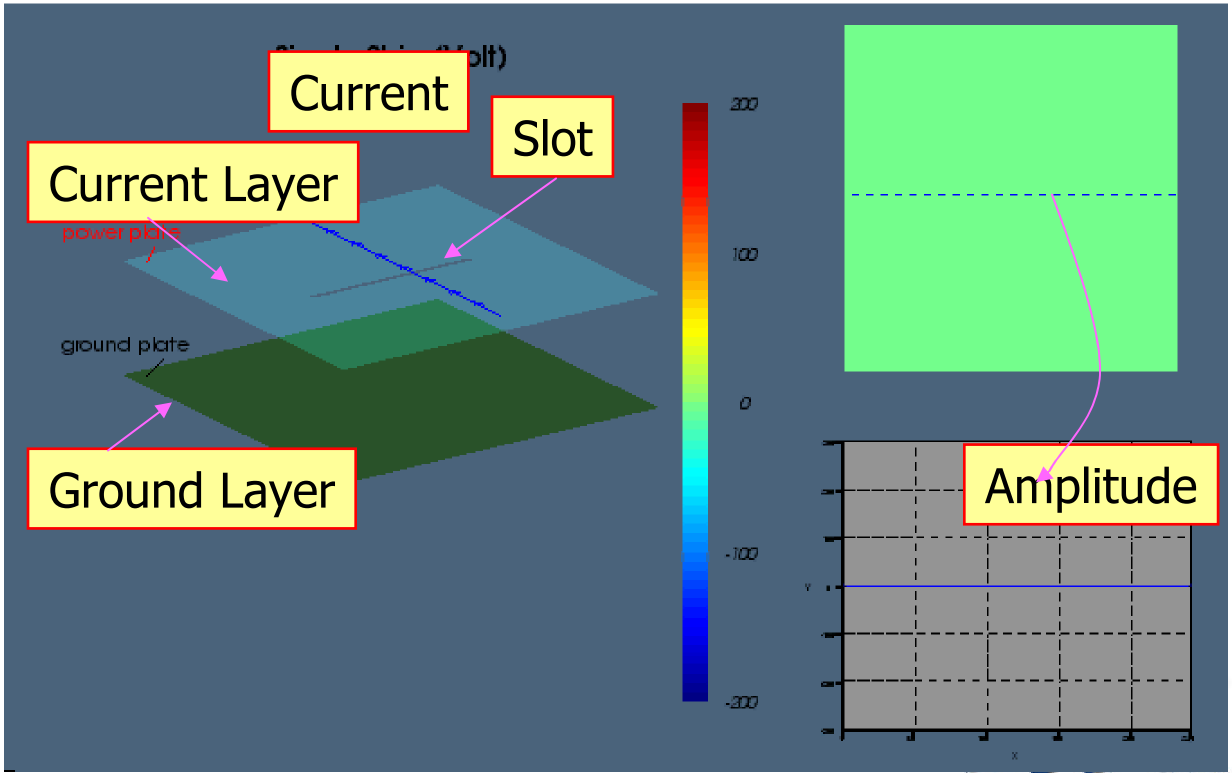


(Data courtesy of Chun-Hao Teng, AnCAD, Inc.)

Multi-layer Ground Noise in a Current Field I

Single microstrip line crossing slot

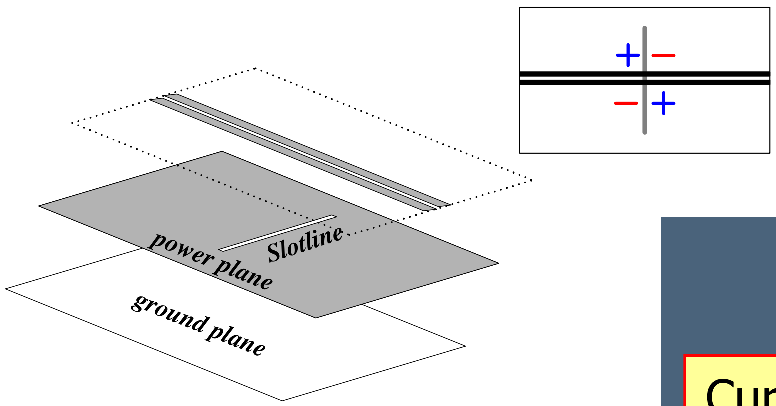


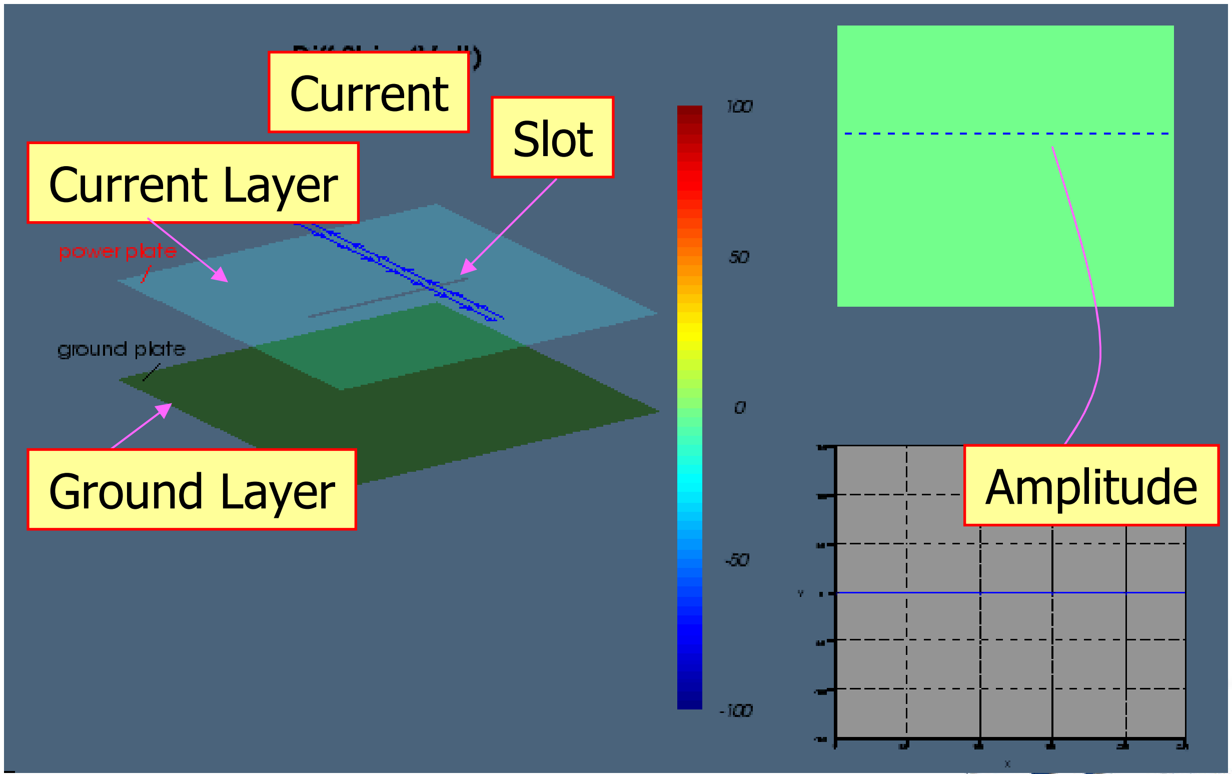


(Data courtesy of Ruey-Beei Wu/Kuang-Hua Hsueh, National Taiwan University)

Multi-layer Ground Noise in a Current Field II

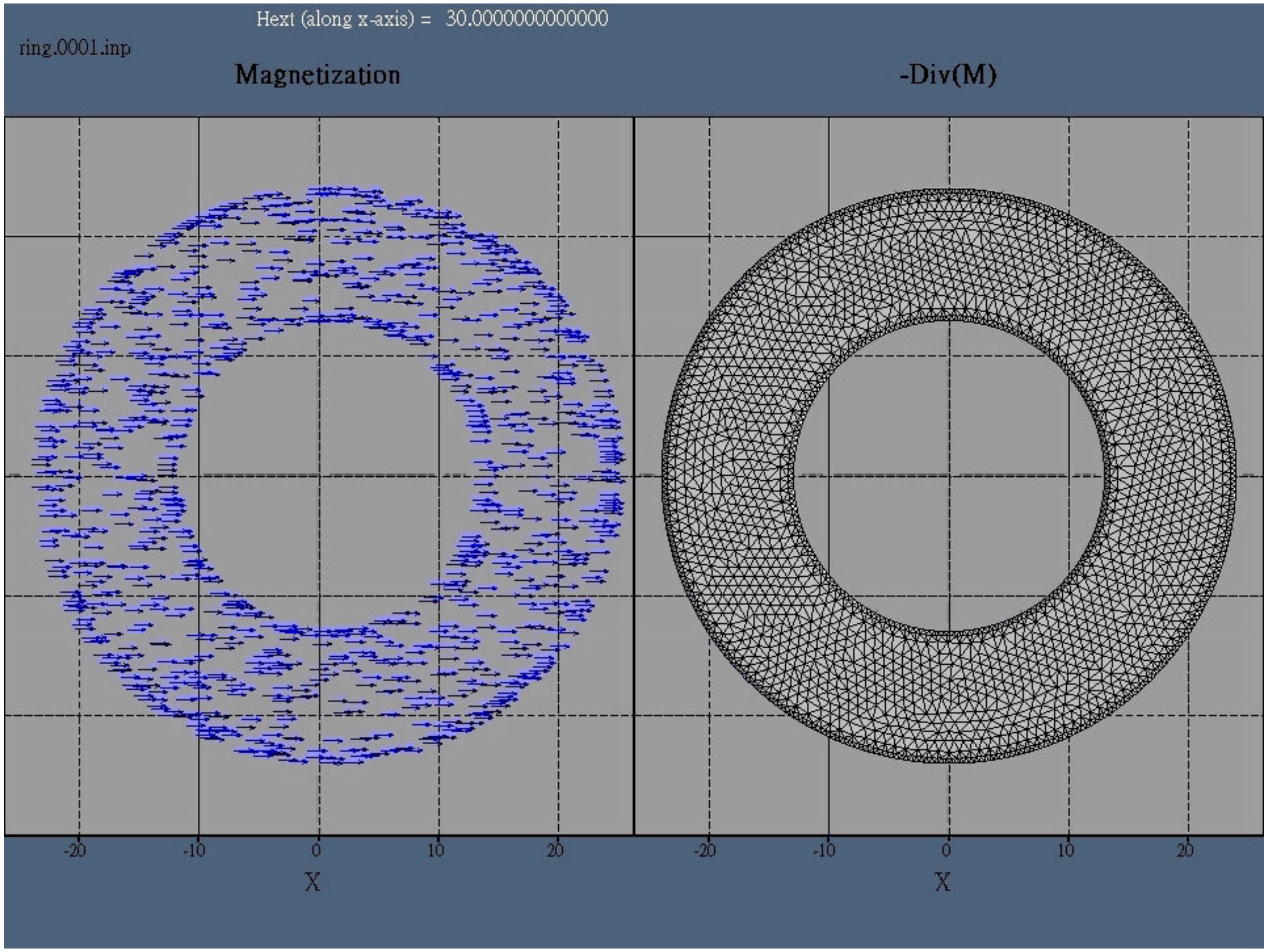
Differential microstrip line crossing slot (coupling factor = 0.305)





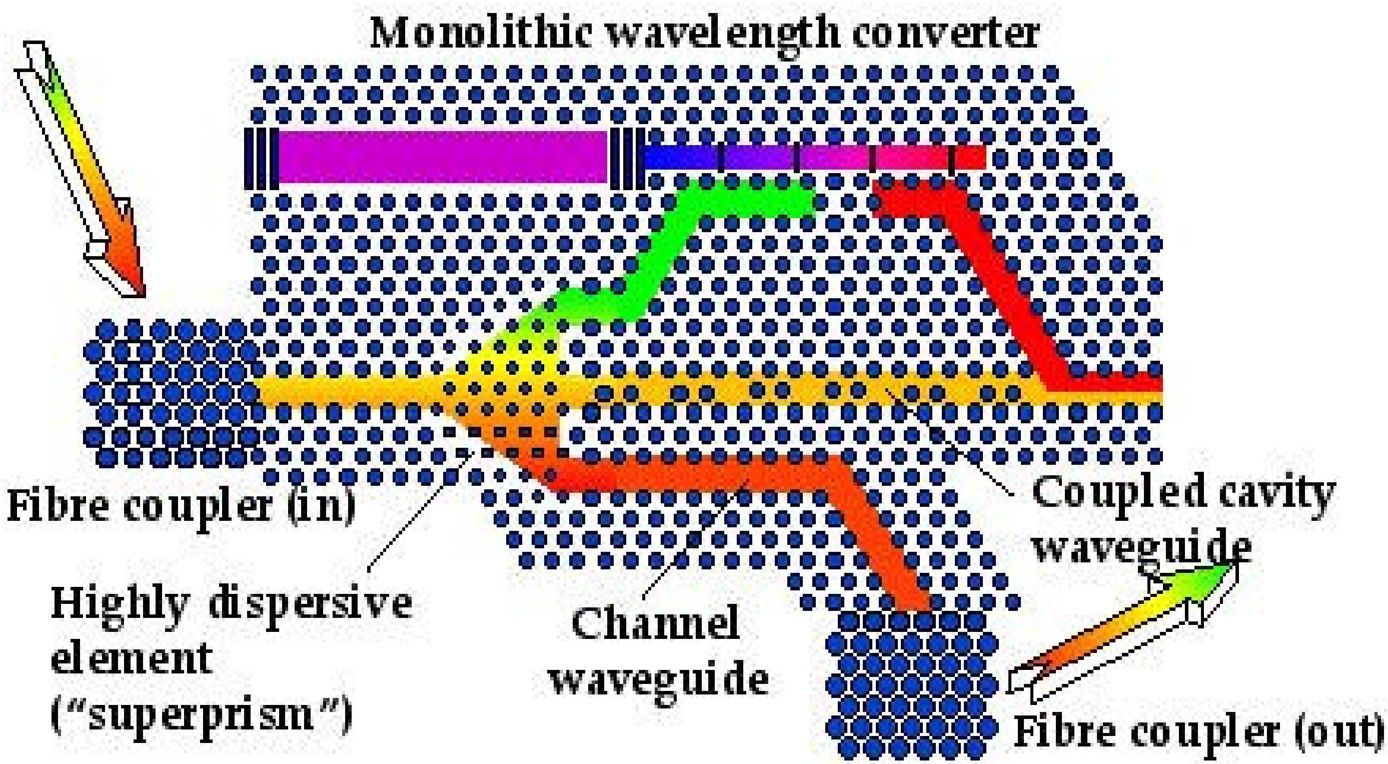
(Data courtesy of Ruey-Beei Wu/Kuang-Hua Hsueh, National Taiwan University)

Micro-magnetic Simulations



(Data courtesy of Professor Lee, Ching-Ming, Chungchou Institute of Technology.)

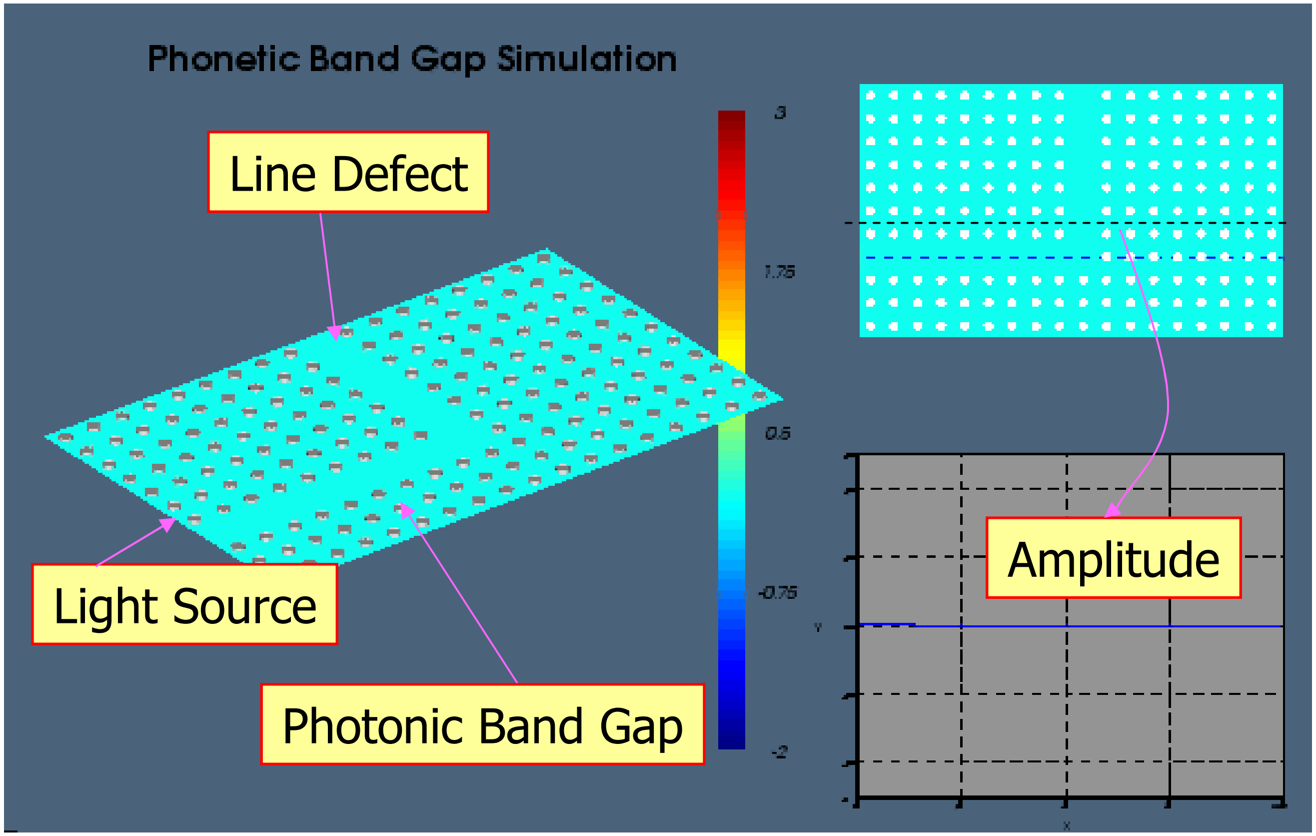
Photonic Band Gap Waveguide Transmission I



The blueprint of future integrated optical circuits.

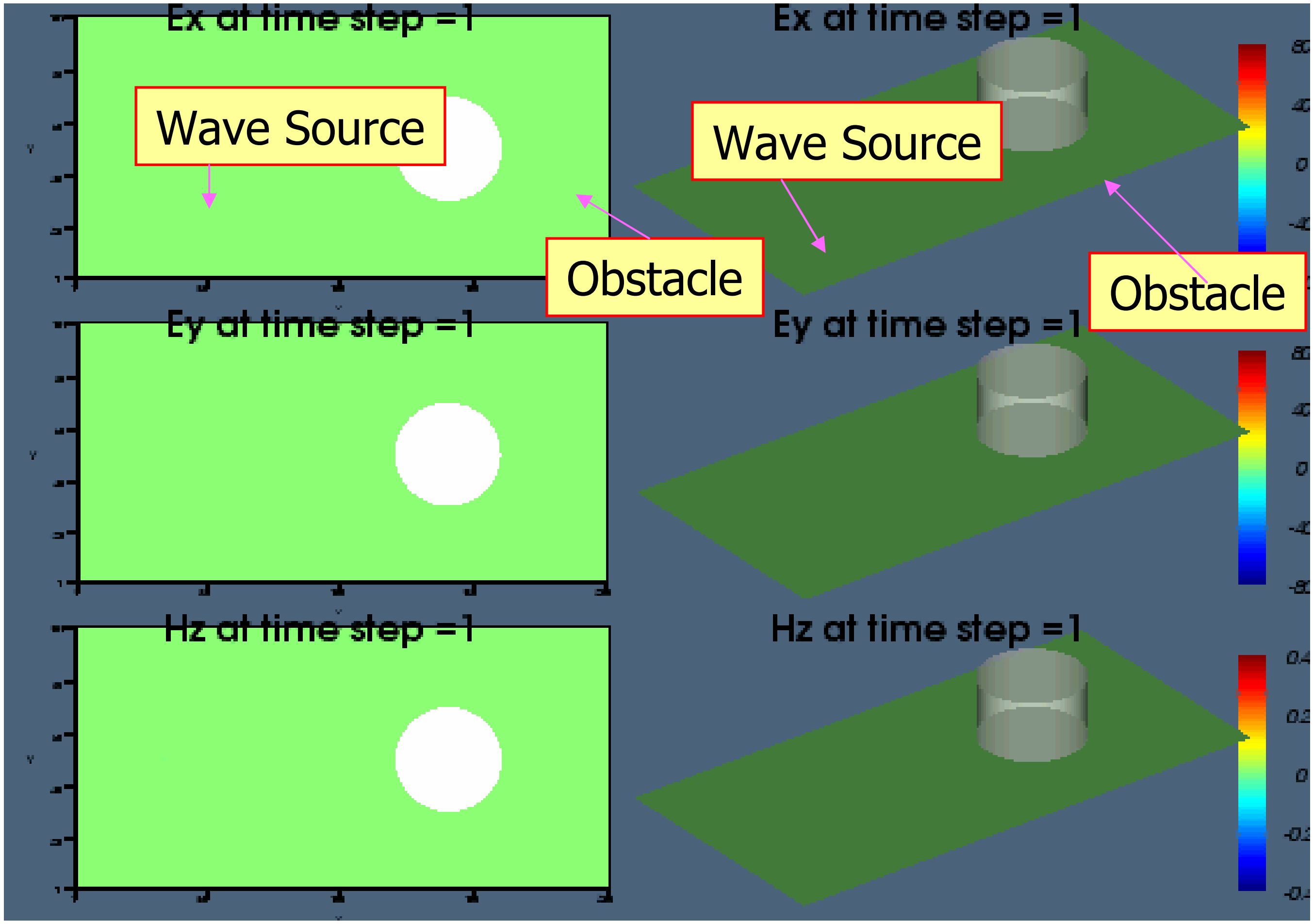
(Data courtesy of Department of Physics & Astronomy, University of St Andrews, UK)

Photonic Band Gap Waveguide Transmission II



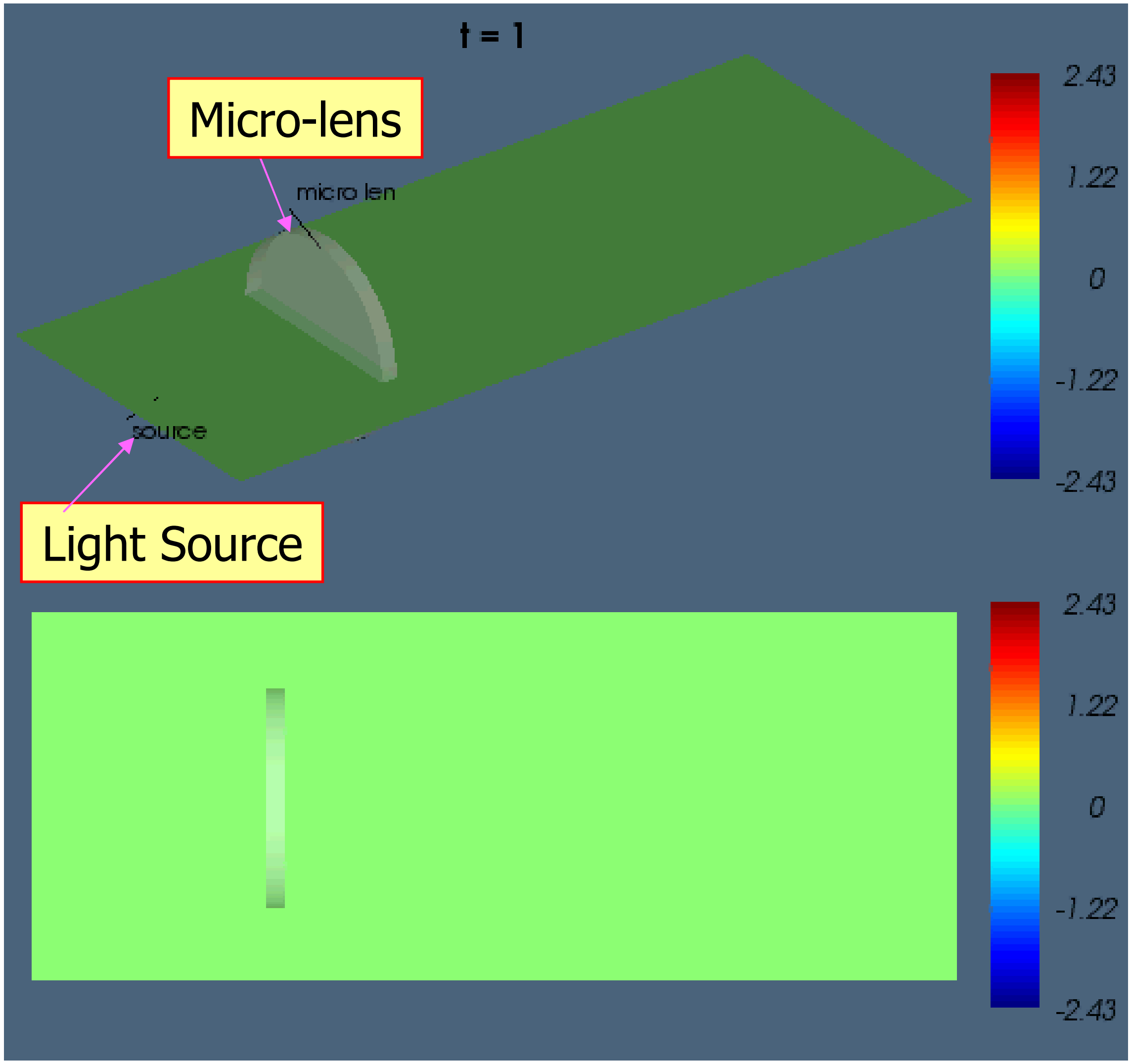
(Data courtesy of Dr. Pei-Kun Wei, Academia Sinica, Taiwan)

Finite-difference Time-domain Analysis



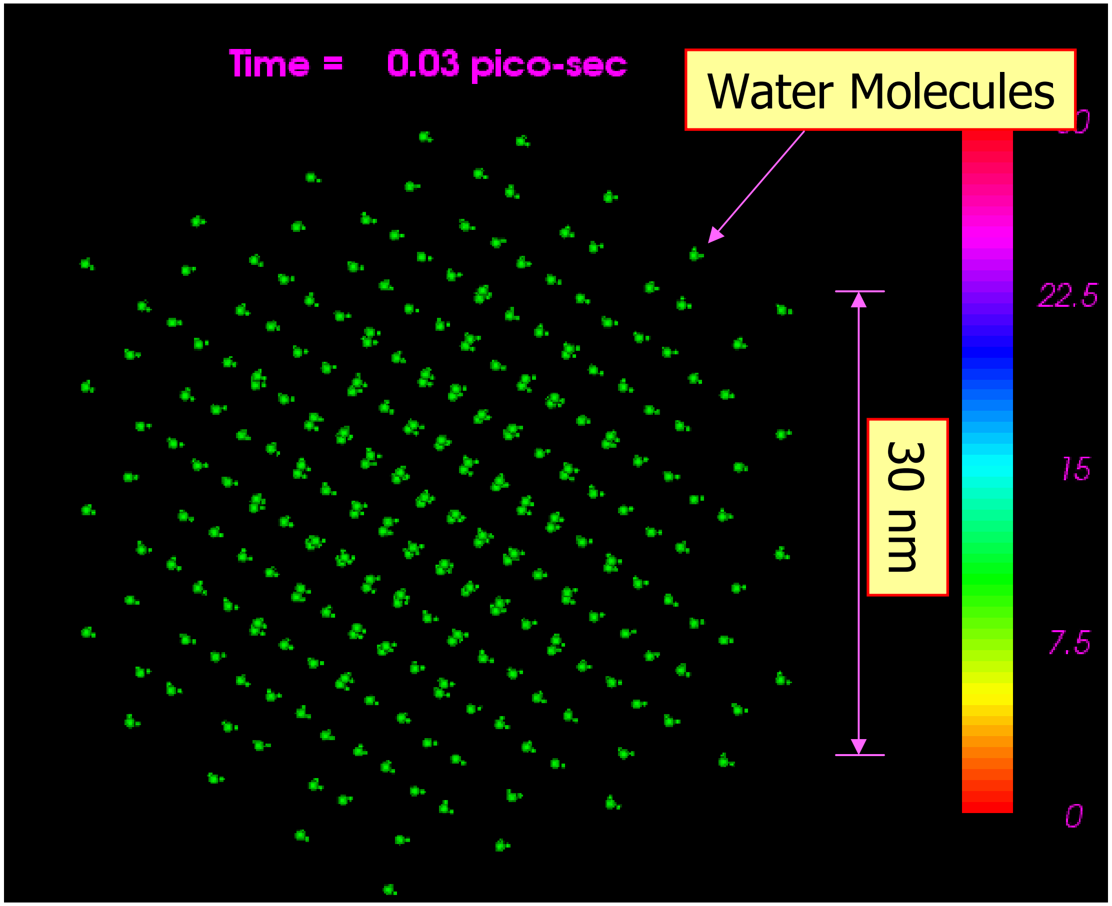
(Data courtesy of Yu-Jen Lin, Precision Instrument Development Center)

Analysis of Optical Thin-film Coated Micro-lens



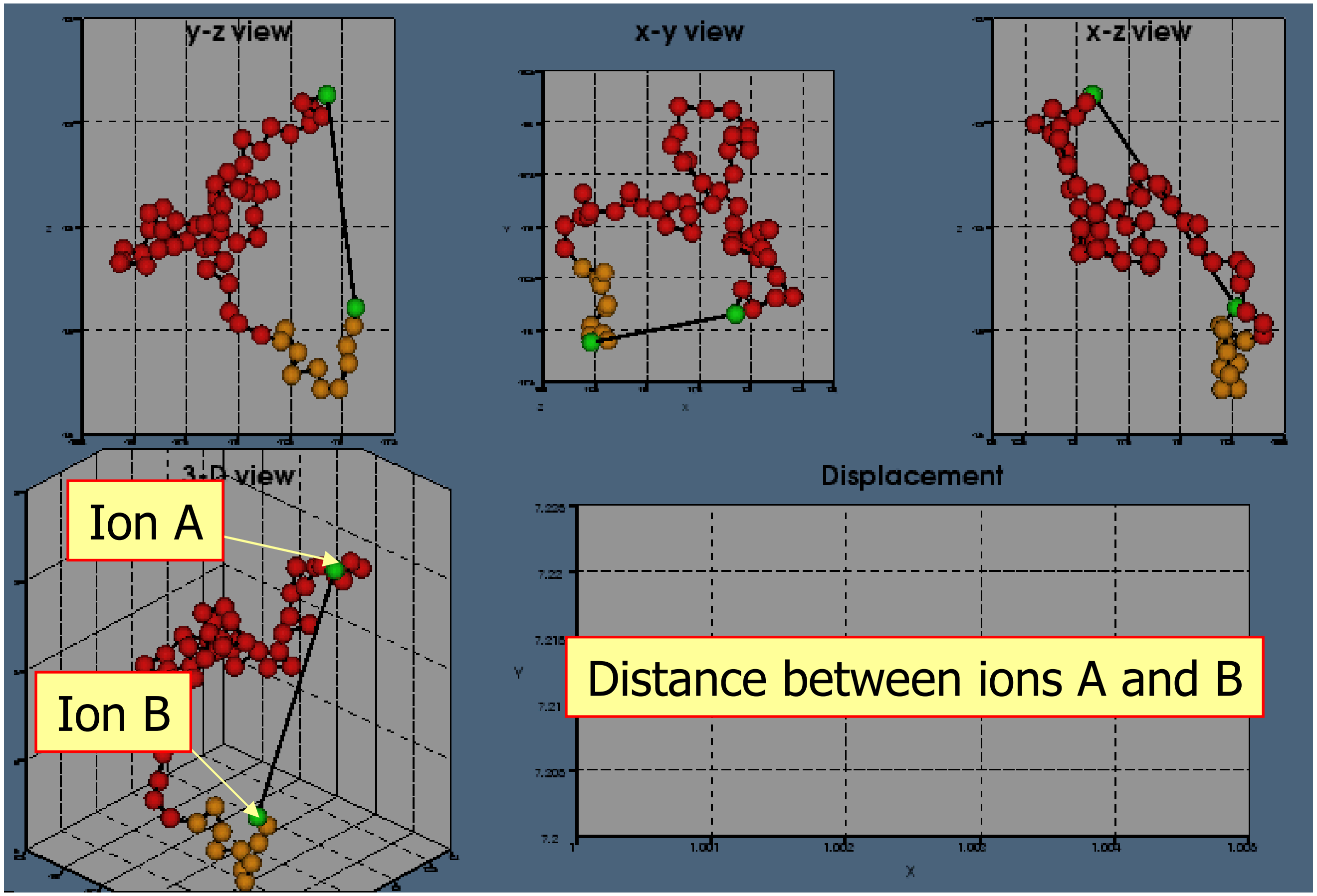
(Data courtesy of Tung-Lung Fu, Precision Instrument Development Center)

Water Molecule Phase Transition



(Data courtesy of Chin-Hsiang Cheng, Tatung University)

Ion Perturbation Analysis



(Data courtesy of Yu-Chang Sheng, National Taiwan University)

Visualization of Physical Problem by **MATFOR®**

Electromagnetic Radiation

- Dipole

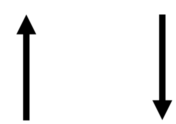
$$\left\langle \vec{S} \cdot \vec{n} \right\rangle = \frac{1}{2} \frac{p_0^2}{4\pi} \frac{\omega^4}{c^3} \sin^2(\theta) \frac{1}{r^2}$$

- Quadrupole

axial separation

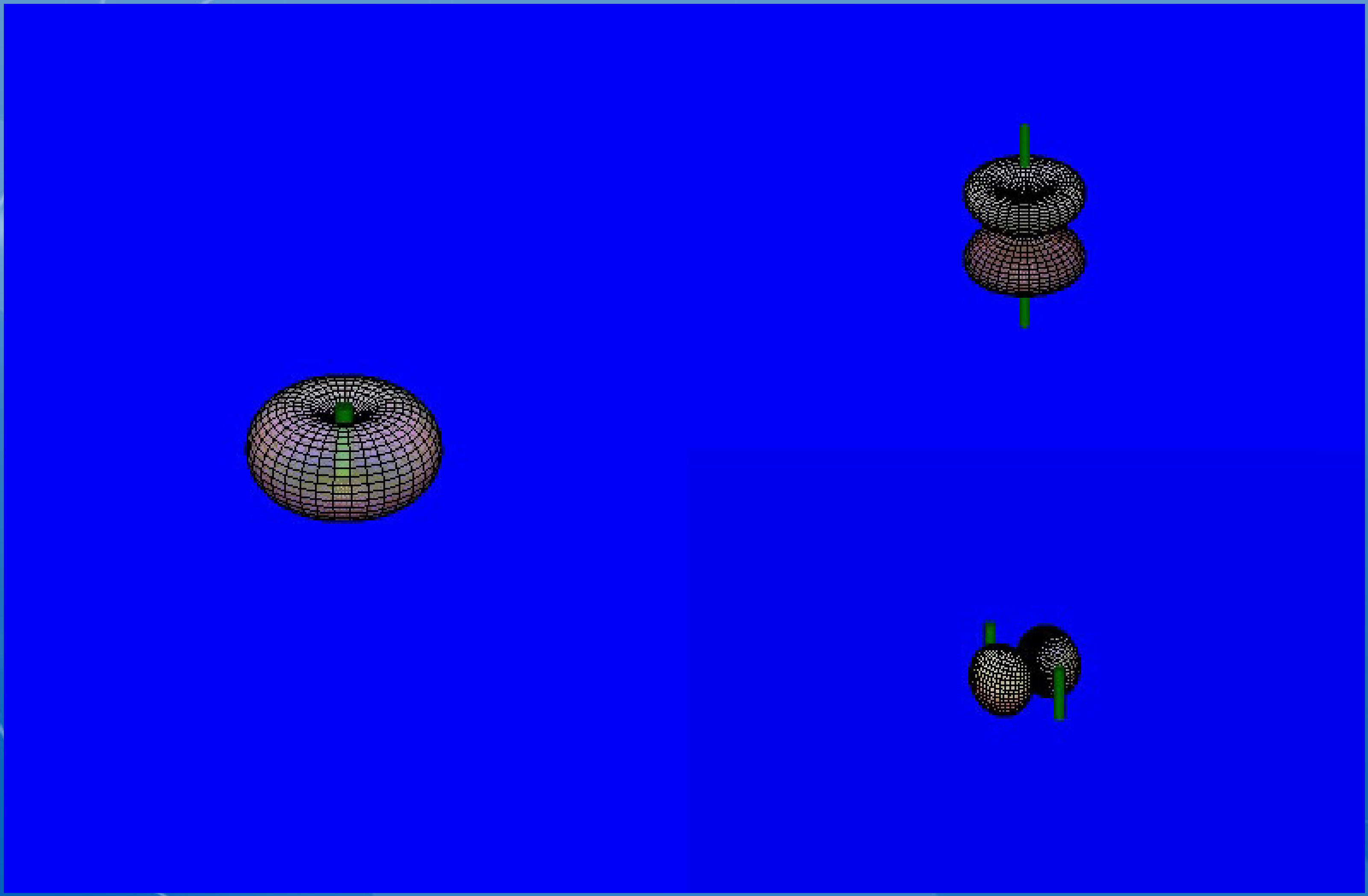
$$\left\langle \vec{S} \cdot \vec{n} \right\rangle = \frac{1}{2} \frac{Q^2}{32\pi^2} \frac{\omega^6}{c^5} \sin^2(\theta) \sin^2\left[kd\cos(\theta)\right] \frac{1}{r^2}$$

laterial separation



$$\left\langle \vec{S} \cdot \vec{n} \right\rangle = \frac{1}{2} \frac{p_0^2}{\pi} \frac{\omega^4}{c^3} \sin^2(\theta) \sin^2\left[\frac{kd}{2} \sin(\theta) \cos(\varphi)\right] \frac{1}{r^2}$$

Visualizing the Radiation Pattern



Diffraction Integral

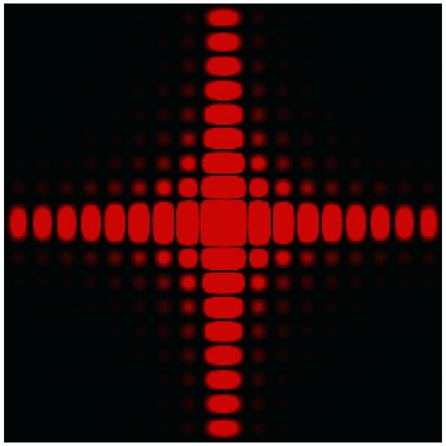
- Fresnel-Kirchhoff :

$$\psi(P) = \frac{1}{i}\frac{\psi_0}{2\lambda}\int_\sigma \frac{e^{ikr}}{r}(1+\cos(\theta))da$$

- Frauhofer :

$$\psi(\alpha,\beta) = \frac{1}{i}\frac{\psi_0 e^{ikR}}{\lambda Z}\int_\sigma e^{-ik(\alpha\xi+\beta\eta)}d\xi d\eta$$

($R >> \lambda >> D \quad \therefore r \approx R(\alpha\xi+\beta\eta)$)



Slit Diffraction

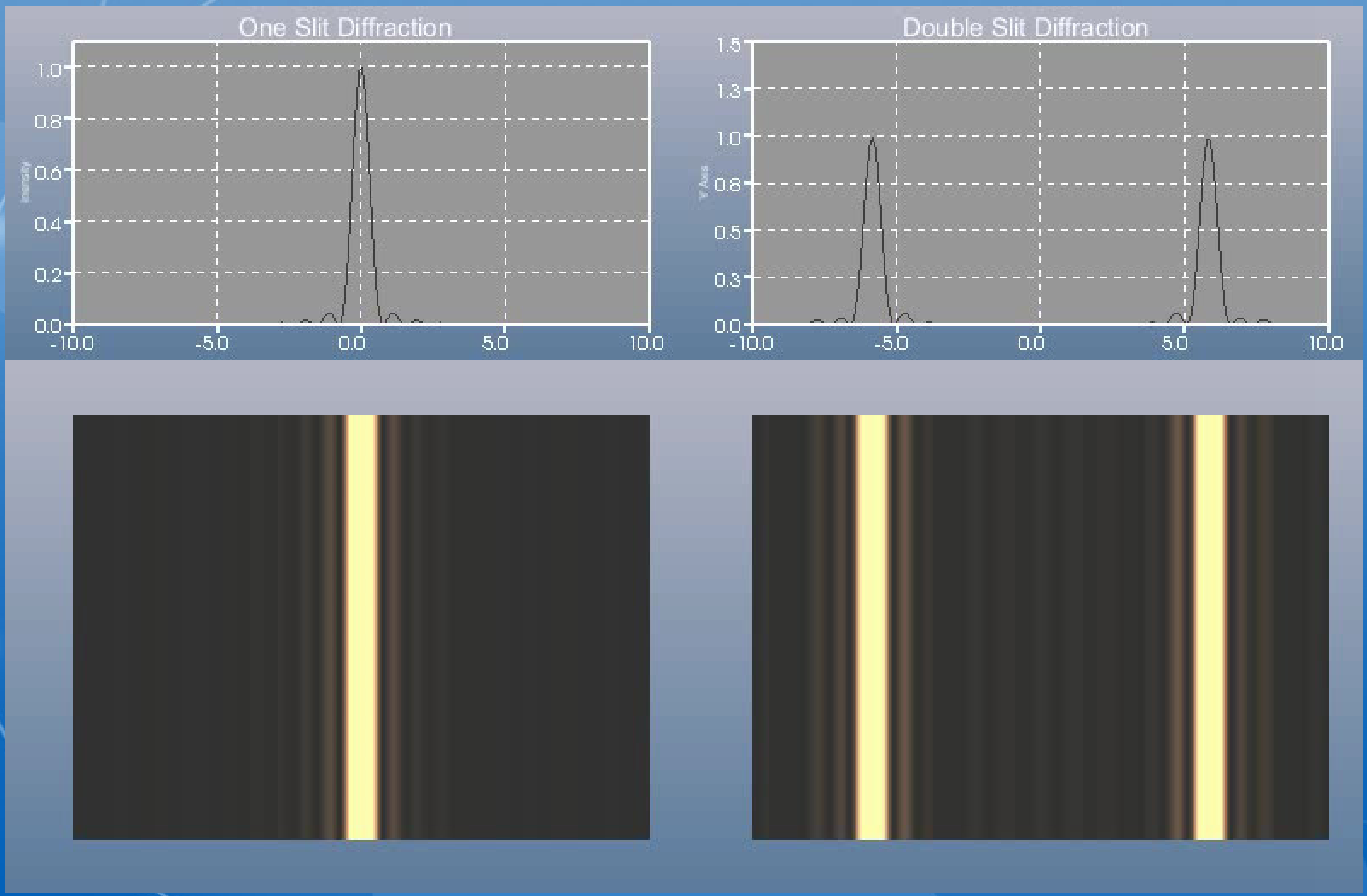
- In one dimensional ,The Fraunhofer Diffraction Integral becomes :

$$\psi(\alpha) = C\int_{\sigma} e^{-ik\alpha\xi} d\xi$$

- If the slit is of width 2a, then the integral is :

$$\psi(\theta) = C\int_{-a}^{a} e^{-ik\alpha\xi} d\xi = \underline{\underline{2Ca(\frac{\sin(u)}{u})}} \quad , u = ka\alpha = \frac{2\pi}{\lambda} a\sin(\theta)$$

Visualization of the Slit Diffraction



Circular Aperture

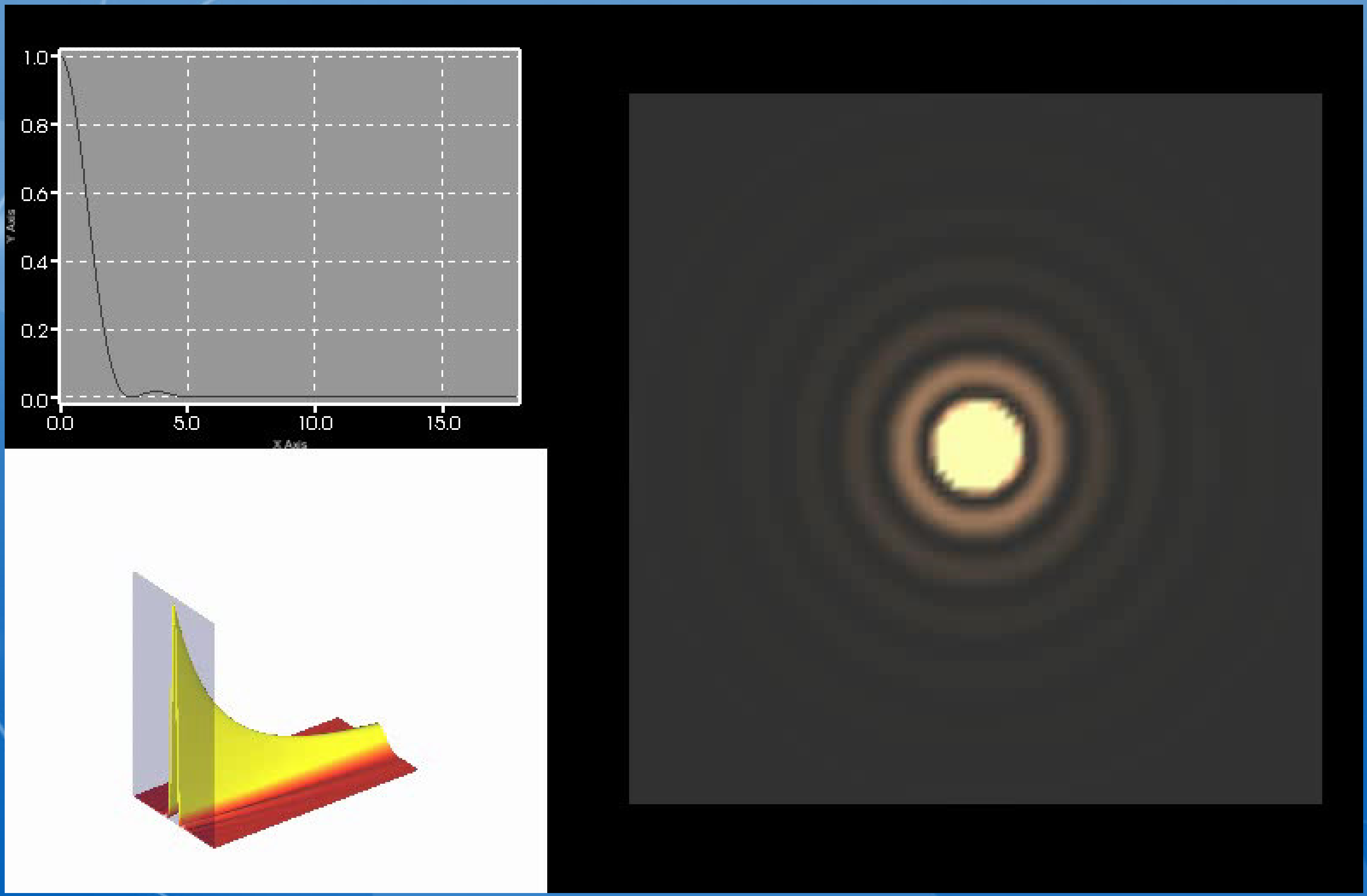
$$\psi(P) = C\int_{\sigma} e^{-ik(\alpha\xi+\beta\eta)}d\xi d\eta \quad \xi = \rho\cos(\varphi), \eta = \rho\sin(\varphi)$$

$$\alpha\xi + \beta\eta = \rho\theta\cos(\varphi - \varphi')$$

$$\therefore \psi(\theta) = C\int_0^a\int_0^{2\pi} e^{-ik\rho\theta\cos\varphi}\rho\cdot d\theta d\rho = 2\pi C\int_0^a J_0(ka\theta)\rho d\rho = 2\pi Ca^2\left(\frac{J_0(u)}{u}\right)$$

$$u = \frac{2\pi}{\lambda}a\theta, \quad \left|\pi a^2 C\right|^2 = \left(\frac{\pi a^2}{Z\lambda}\right)\left|\psi_0\right|^2$$

Visualizing the Circular-Aperture Diffraction



Optical Soliton : Kerr Effect

This refractive index variation is responsible for the nonlinear optical effects of self-focusing and self-phase modulation, and is the basis for Kerr-lens modelocking.

Type Kerr effect:

$$n = n_0 + n_2 I$$

Slow Vary Approximation

$$\nabla^2 E + n^2 k_0^2 E = 0, \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}$$

$$\left[\frac{\partial^2 a}{\underline{\underline{\partial z^2}}} + i(2n_0 k_0) \cdot \frac{\partial a}{\partial z} + (-1)(n_0 k_0)^2 + \frac{\partial^2 a}{\partial x^2} \right] + (nk_0)^2 a = 0$$

$$for \quad k \sim \frac{1}{\lambda} \quad , \Delta z >> \lambda \quad \rightarrow \left| k_0 \frac{\partial a}{\partial z} \right| >> \left| \frac{\partial^2 a}{\partial z^2} \right|$$

$$and \quad n^2 - n_0^2 = (n - n_0)(n + n_0) \approx (2n) n_0 I$$

$$eq. \Rightarrow \frac{\partial a}{\partial z} = i \frac{1}{2n_0 k_0} \frac{\partial^2 a}{\partial x^2} + i\left(\frac{n_0 k_0 n^2}{2} |a|^2\right) \cdot a$$

$$set \quad \frac{1}{2n_0 k_0} \equiv \alpha, \quad \frac{n_0 k_0 n^2}{2} \equiv \beta$$

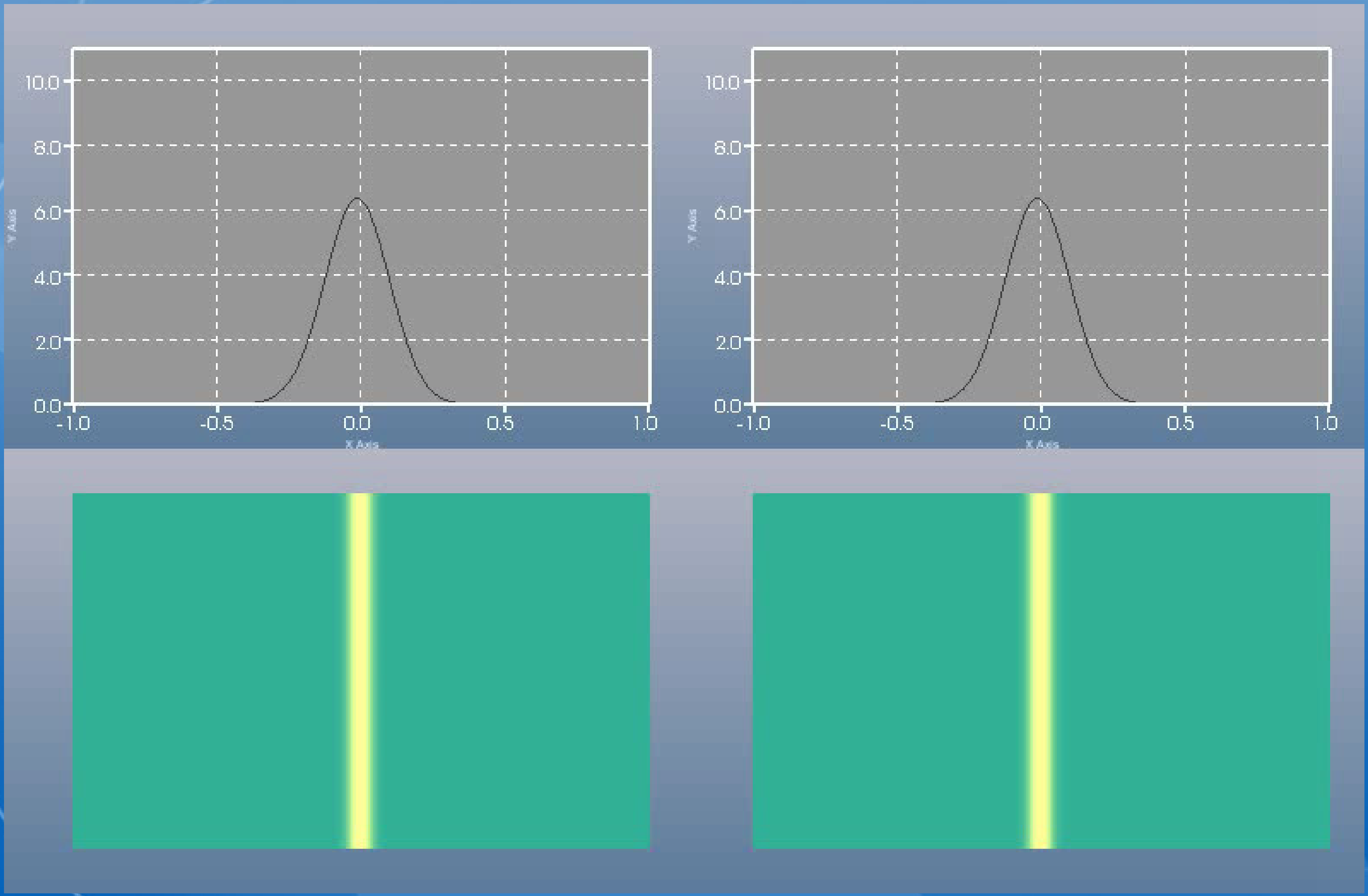
Split Step Fourier Method

$$\frac{\partial a}{\partial z} = i\alpha \frac{\partial^2 a}{\partial x^2} + i(\beta |a|^2) \cdot a$$

$$\Rightarrow \frac{\partial a}{\partial z} = \left(\hat{L} + \hat{N}\right) a \quad \Rightarrow a = e^{(\hat{L}+\hat{N})z} a_0 \approx e^{\hat{L}\cdot z} e^{\hat{N}\cdot z} a_0$$

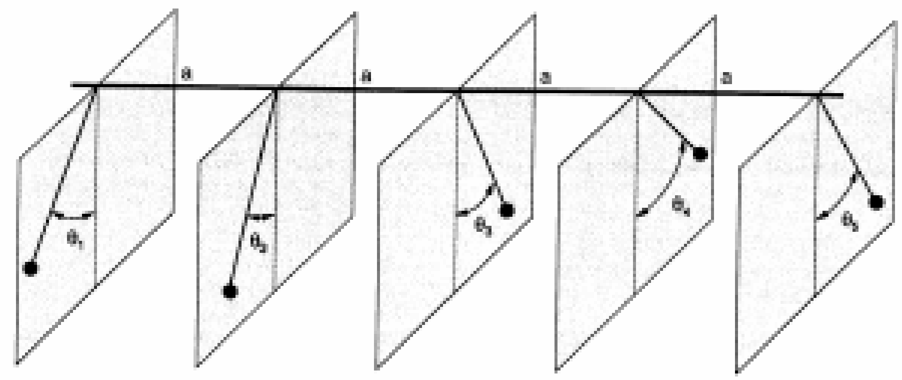
$$\Rightarrow \underline{\underline{a_{n+1} = e^{i\alpha(-k^2)\cdot \Delta z} F[e^{i\beta |a|^2} a_n]}}$$

SSF simulation result for Kerr soliton.



Sin-Gordon Equation

- Considing a 1-D chan of identiacl pendu;la connenected by a torsion bar.



- The euqation of motion for pendulum j follows from Newton's law for rotational motion in terms of torques:

$$\sum_{j \neq i} \tau_{ji} = I\alpha_j$$

$$-\kappa(\theta_j - \theta_{j-1}) - \kappa(\theta_j - \theta_{j+1}) - mg\sin(\theta) = I\,\frac{d^2\theta_j(t)}{dt^2}$$

2D Sin-Gordon Equation

- If the wavelength in a pulse are much longer than the repeat disance a, the chain could be approximated as a continuous medium.

$$\theta_{j+1} \approx \theta_j + \frac{\partial \theta}{\partial x} \cdot a$$

$$-(\theta_j - \theta_{j-1}) - (\theta_j - \theta_{j+1}) \approx \frac{\partial^2 \theta}{\partial x^2} \cdot (a)^2$$

$$\Rightarrow \lim_{a \to 0} \frac{\partial^2 \theta}{\partial t^2} - \frac{\kappa a}{I} \frac{\partial^2 \theta}{\partial x^2} = \frac{mg}{I} \sin(\theta)$$

- Then generalizing the spatial derivatives:

$$\nabla^2 \theta - \alpha \cdot \frac{\partial^2 \theta}{\partial x^2} = \beta \cdot \sin(\theta)$$

Sin-Gordon Equation: 1D solution

1-D analytic solution :

$$\frac{\partial^2 \theta}{\partial t^2} - \frac{\partial^2 \theta}{\partial x^2} = \sin(\theta) \quad , \theta(x,t)$$

$$\xi = t \pm \frac{x}{v}$$

$$\frac{d^2 \theta}{d \xi^2} = \frac{v^2}{v^2 - 1} \sin(\theta)$$

$$for \quad v \sim \pm 1$$

$$\theta(x - vt) = \begin{cases} 4 \tan^{-1}\left[\exp\left[\frac{x - vt}{(1 - v^2)^{\frac{1}{2}}}\right]\right] \\ 4 \tan^{-1}\left[\exp\left[-\frac{x - vt}{(1 - v^2)^{\frac{1}{2}}}\right]\right] + \pi \end{cases}$$

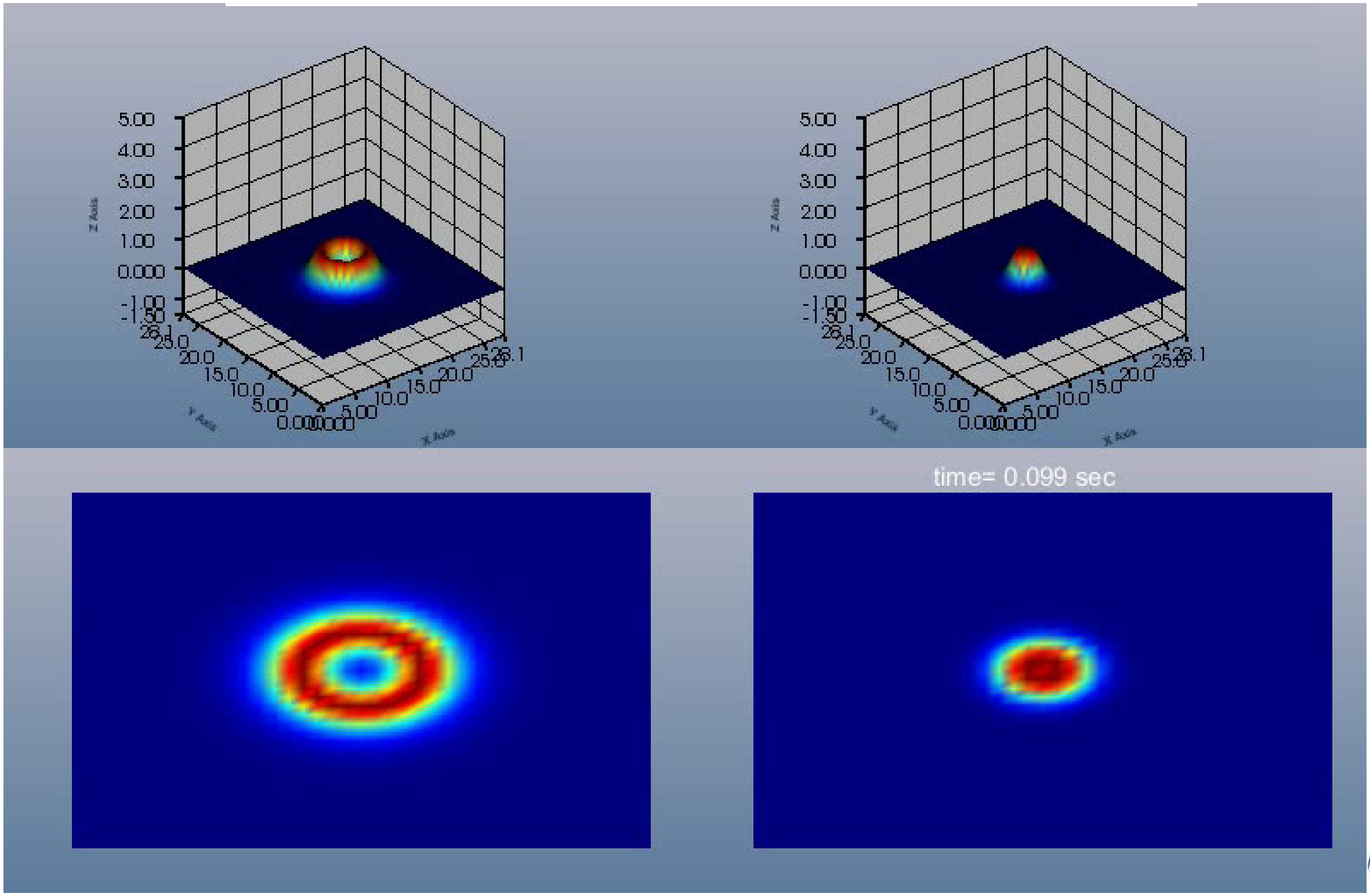
So the 2D initial gauss be :

$$\theta(x, y, t = 0) = 4 \tan^{-1}\left[\exp\left(c - \left(x^2 + y^2\right)^{\frac{1}{2}}\right)\right]$$

where c be some constant.

2D Dynamical Sin-Gordon Equation

Initial condition, left: above equation; right: Gaussian form.



Quantum bound

- In multiple-particle nature, the interaction leads the nonlocal potential :. It changes the interaction term in Schrodinger equation :

$$V(r)\psi(r) \rightarrow \int V(r,r')\psi(r')dr'$$

- Then the equation becomes :

$$H\psi = E\psi$$

$$\frac{p^2}{2\mu}\psi_n(k) + \frac{2}{\pi}\int_0^{\infty} V(p,k)\psi_n(k)p^2 dp + E_n\psi_n(k)$$

- One way to deal with the equation is by going to k-space(Bessel transformation):

$$\frac{p^2}{2\mu}\psi_n(k)+\frac{2}{\pi}\int_0^\infty V(p,k)\psi_n(k)\,p^2dp+E_n\psi_n(k)$$

the k-space potential is obtain by a double Bessel transform

$$(2\pi)^3\int_0^\infty\left(\int_0^\infty j_l(kr')V(r,r')r'dr\right)j_l(pr)rdr=(2\pi)^3\int_0^\infty j_l(kr)V(r)j_l(pr')r^2dr$$

Numerically, The Schrodinger equation be :

$$\frac{k^2}{2\mu}\psi_n(k)+\frac{2}{\pi}\sum_{i=1}^{N}k_j^2V(k,k_j)\Delta k_j\cdot\psi_n(k_j)=E_n\psi_n(k)$$

- In matrix form :

$$[H]\cdot[\psi_n] = E_n[\psi_n] \quad H_{ij} = \frac{k_i^2}{2\mu}\delta_{ij} + \frac{2}{\pi}V(k_i, k_j)k_j^2\Delta k_j$$

$$[\psi_n] = \begin{pmatrix} \psi_n(k_1) \\ \psi_n(k_2) \\ \vdots \\ \psi_n(k_N) \end{pmatrix}$$

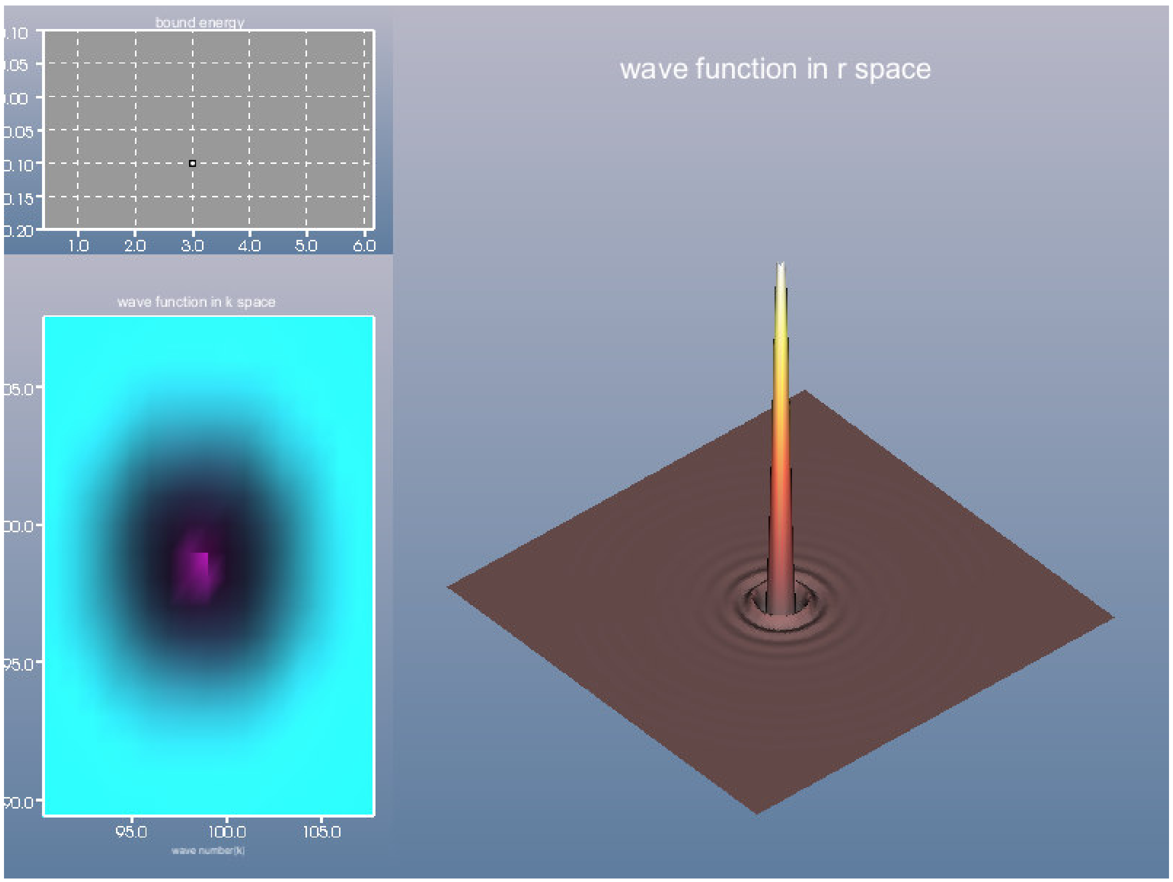
- To solve the eigensystem problem, we could receive several eigenvalues, but only one satisfys $|H - E_n I|$ (boundary condition). Once we find the $\psi(k)$, by inverse Bessel transformation we could get the wave function in r-space without any difficault : .

$$\psi(r) = \int_0^\infty \psi_n(k) j_l(kr) k^2 dk$$

$$V(r) = \frac{\lambda}{2\mu}\delta(r-b)$$

The simplest case : $V(r) = \frac{\lambda}{2\mu}\delta(r-b),\qquad V(k,p) = \int_0^\infty j_l(kr)V(r)j_l(pr)r^2dr = \frac{\lambda b^2}{2\mu}j_l(kr)j_l(pr)$

.



Summary :MATFOR Components

- **mfArray**
  - integrates the entire MATFOR toolkit into high-level programming environments such as C++ and Fortran, simplifying the syntax and facilitating object-oriented programming.
  - Basic data structure.
- **Numerical Library**
  - contains useful linear algebraic functions subject to assist users with computational problem solving.
  - Use mfArray to do numerical computation
- **Visualization Library**
  - collects well-designed graphical procedures and controls to support a variety of 2D and 3D visual functions.

MATFOR Components (Cont)

- **Data Viewer**
  - organized in spreadsheet format, is one convenient platform for data management, filter, and analysis.
- **Graphics Viewer**
  - besides its highly customized user interface, overthrows the convention of post-processing as it instantly visualizes scientific and engineering data.
- **mfPlayer**
  - captures picture frames, animates simulation results, and allows additional graphical manipulations.

- MATFOR®-

A Simple Yet Powerful Solution to Meet Your Needs!