NOVEL NUMERICAL TECHNIQUES FOR PROBLEMS IN ENGINEERING SCIENCE

Francesco Fedele

(to the memory of my father 1942-2002)

PHYLOSOPHY OF THINKING

PUSH ANALYTICS AS MUCH AS YOU CAN

AND THEN USE NUMERICS

$$\Phi_m(r,\theta,\phi) = \sum \exp(im\theta) P_n^m(\phi) \left[\frac{\partial f}{\partial r} \frac{J_{n+1/2}(\sqrt{-k_m / D_m}\, r)}{\sqrt{r}} - \frac{\beta / D_m}{k_x / D_x - k_m / D_m} \frac{\partial f}{\partial \phi} \frac{J_{n+1/2}(\sqrt{-k_x / D_x}\, r)}{\sqrt{r}} \right]$$

$$\left(\frac{\partial f}{\partial r} \right)_{i-1} \cong \frac{-3u_{i-1} + 4u_i - u_{i+1}}{2\,\Delta r}$$

$$\left(\frac{\partial f}{\partial \phi} \right)_{i} \cong \frac{u_{i+1} - u_{i-1}}{2\Delta \phi}$$

COLLOCATION METHODS
diffusion-advection problems

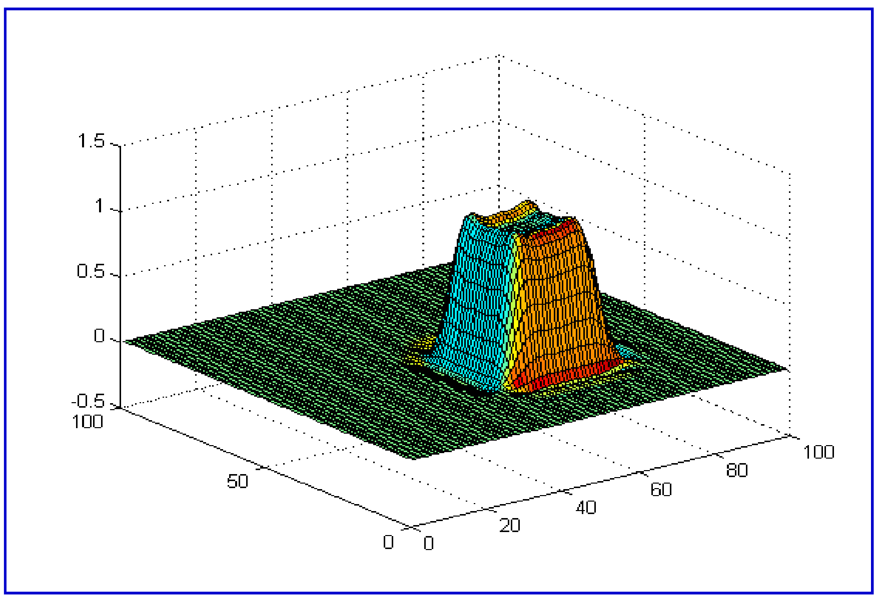
ADJOINT METHODS
Optical tomography

GALERKIN METHODS
Hydrodynamics stability of pipe flows

BOUNDARY ELEMENT METHODS
Photon migration equations

A SINGLE-DEGREE-OF -FREEDOM COLLOCATION SOLUTION TO THE TRANSPORT EQUATION

(LOCOM   LOcalized COllocation Method)



1D ADVECTION-DIFFUSION EQUATION

$$\begin{cases} \mathcal{L}(u) = 0 \\ u(x, t=0) = u_0(x) \\ u(0,t) = 0 \quad u(l,t) = 0 \end{cases}$$

$$u_0(x) \in L_2[0,l]$$

$$\mathcal{L} = \frac{\partial}{\partial t} + c\frac{\partial}{\partial x} - D\frac{\partial^2}{\partial x^2}$$

Advective-diffusive operator

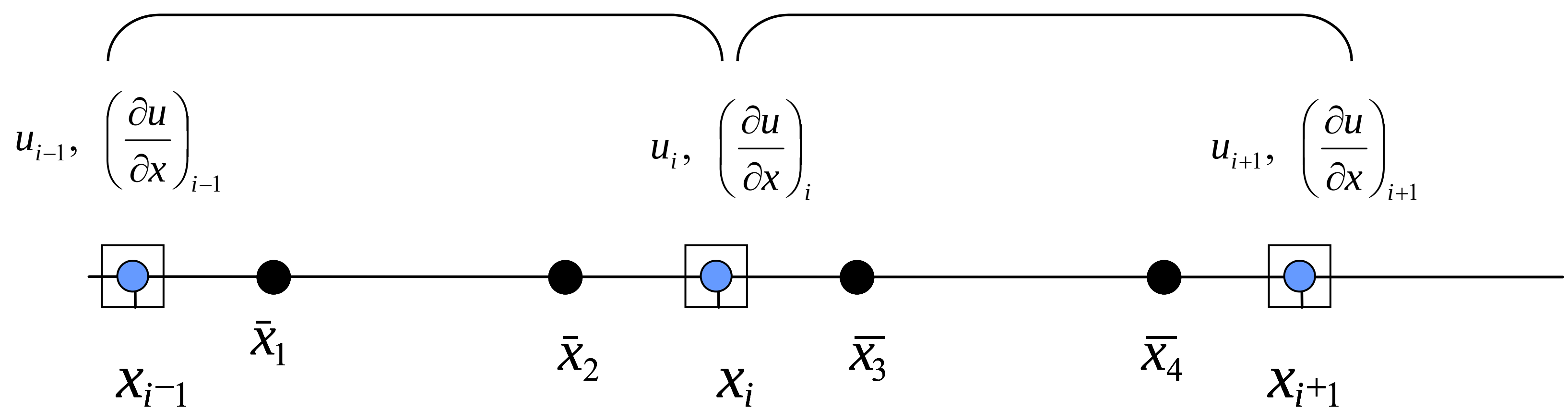
- *u(x,t)* concentration at location *x* at the time *t*
-*c* velocity field
-*D* diffusion coefficient

HERMITE COLLOCATION

Collocation points ● *nodes* ▣

$$\hat{u}(x) \cong \mathcal{H}_{0,i-1}(x)\,u_{i-1} + \mathcal{H}_{1,i}(x)\,u_i + \frac{\Delta x}{2}\overline{\mathcal{H}}_{0,i-1}(x)\left(\frac{\partial u}{\partial x}\right)_{i-1} + \frac{\Delta x}{2}\overline{\mathcal{H}}_{1,i}(x)\left(\frac{\partial u}{\partial x}\right)_{i}$$

$$\hat{u}(x) \cong \mathcal{H}_{0,i}(x)\,u_{i} + \mathcal{H}_{1,i+1}(x)\,u_{i+1} + \frac{\Delta x}{2}\overline{\mathcal{H}}_{0,i}(x)\left(\frac{\partial u}{\partial x}\right)_{i} + \frac{\Delta x}{2}\overline{\mathcal{H}}_{1,i+1}(x)\left(\frac{\partial u}{\partial x}\right)_{i+1}$$

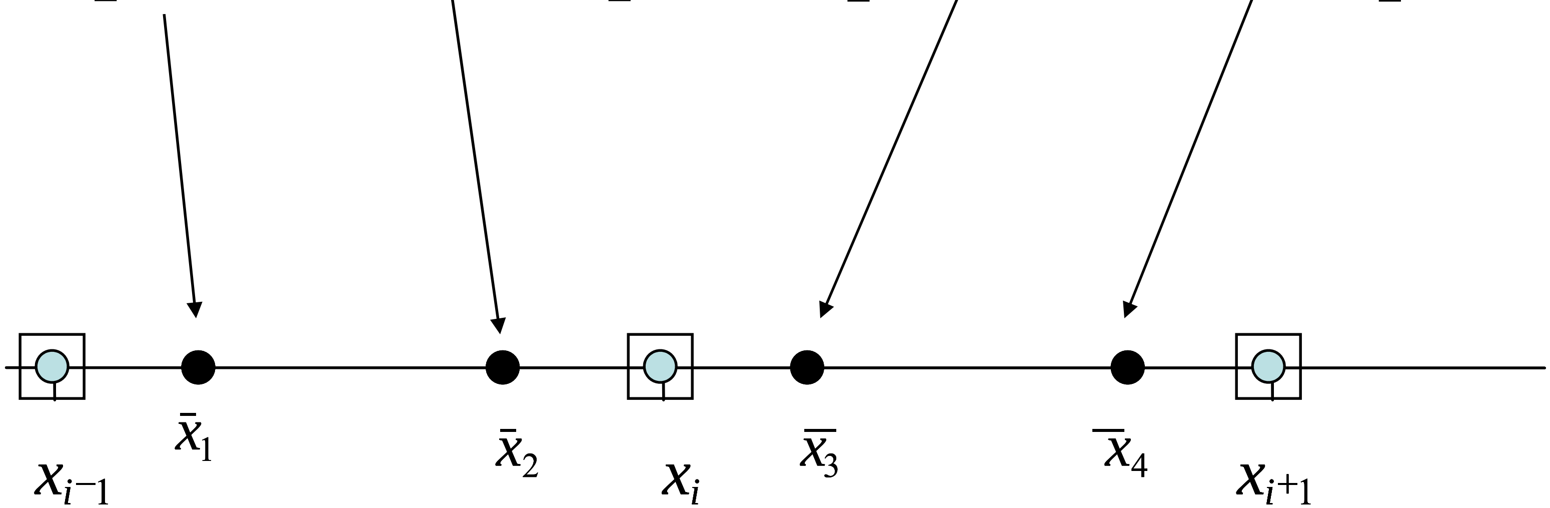


$$\left(\frac{\partial u}{\partial x}\right)_{i-1} \cong \frac{-3u_{i-1} + 4u_i - u_{i+1}}{2\Delta x} \qquad \left(\frac{\partial u}{\partial x}\right)_{i} \cong \frac{u_{i+1} - u_{i-1}}{2\Delta x} \qquad \left(\frac{\partial u}{\partial x}\right)_{i+1} \cong \frac{u_{i-1} - 4u_i + 3u_{i+1}}{2\Delta x}$$

WEIGHTED STRATEGY

Defintion of the semi-discrete operator at the generic node

$$\hat{\mathcal{L}}_x(u)_i = \beta\frac{1}{2}\left[\ \mathcal{L}\left(U^L\right)\Big|_{\bar{x}_1} + \mathcal{L}\left(U^L\right)\Big|_{\bar{x}_2}\ \right] + (1-\beta)\,\frac{1}{2}\left[\ \mathcal{L}\left(U^R\right)\Big|_{\bar{x}_3} + \mathcal{L}\left(U^R\right)\Big|_{\bar{x}_4}\ \right]$$



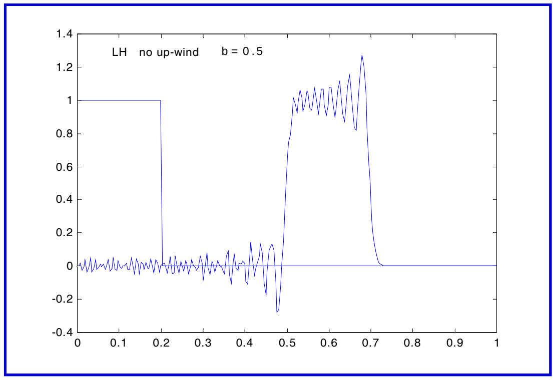
$\beta \quad up-wind \;\; parameter$

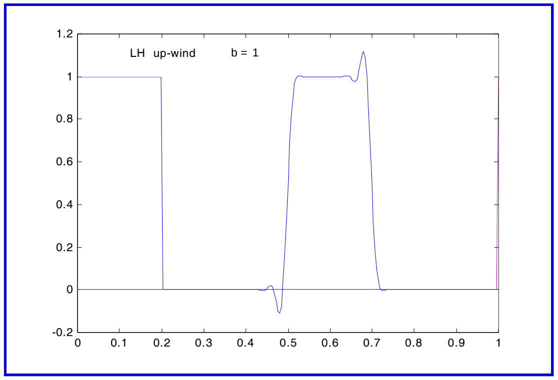
SEMI-DISCRETE SPATIAL APPROXIMATION

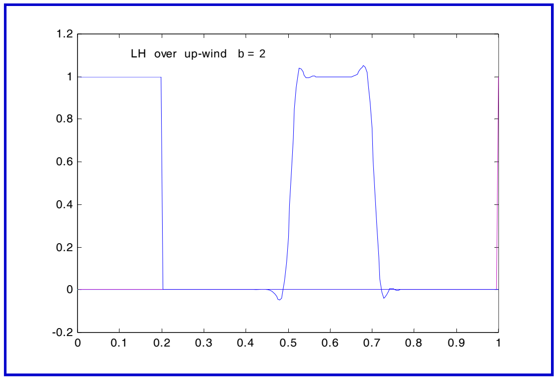
By imposing the vanishing of the discrete operator at each node the following ODE system is achieved

$$a_1 \frac{du_{i-1}}{dt} + a_2 \frac{du_i}{dt} + a_3 \frac{du_{i+1}}{dt} + b_1 u_{i-1} + b_2 u_i + b_3 u_{i+1} = 0 \qquad \forall i = 1,2,..,N_X$$

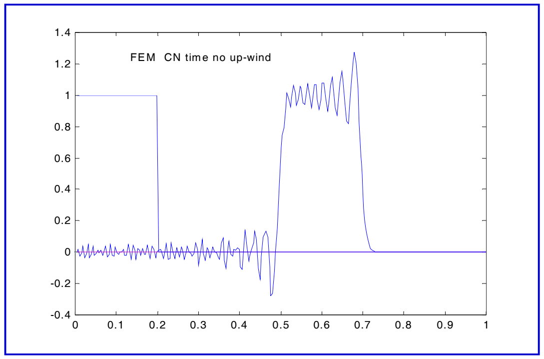
1D SIMULATIONS

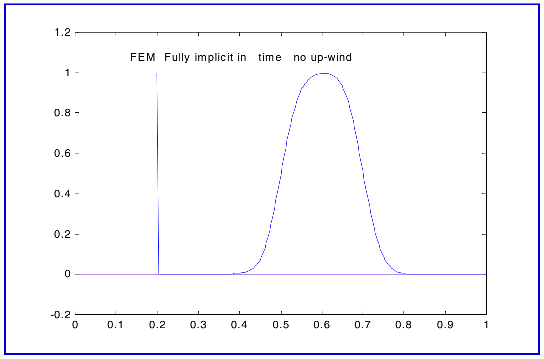


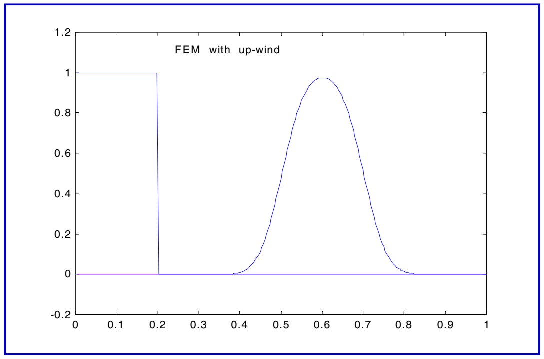




LOCOM from the left side CN in time, full implicit in time, with up-winding

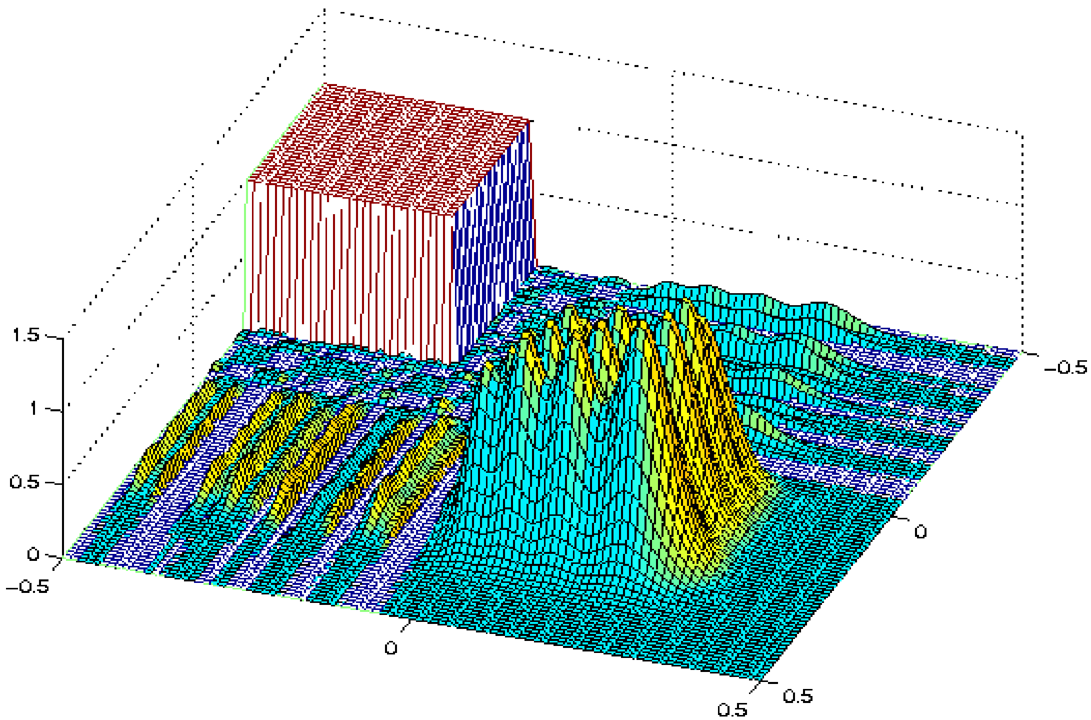




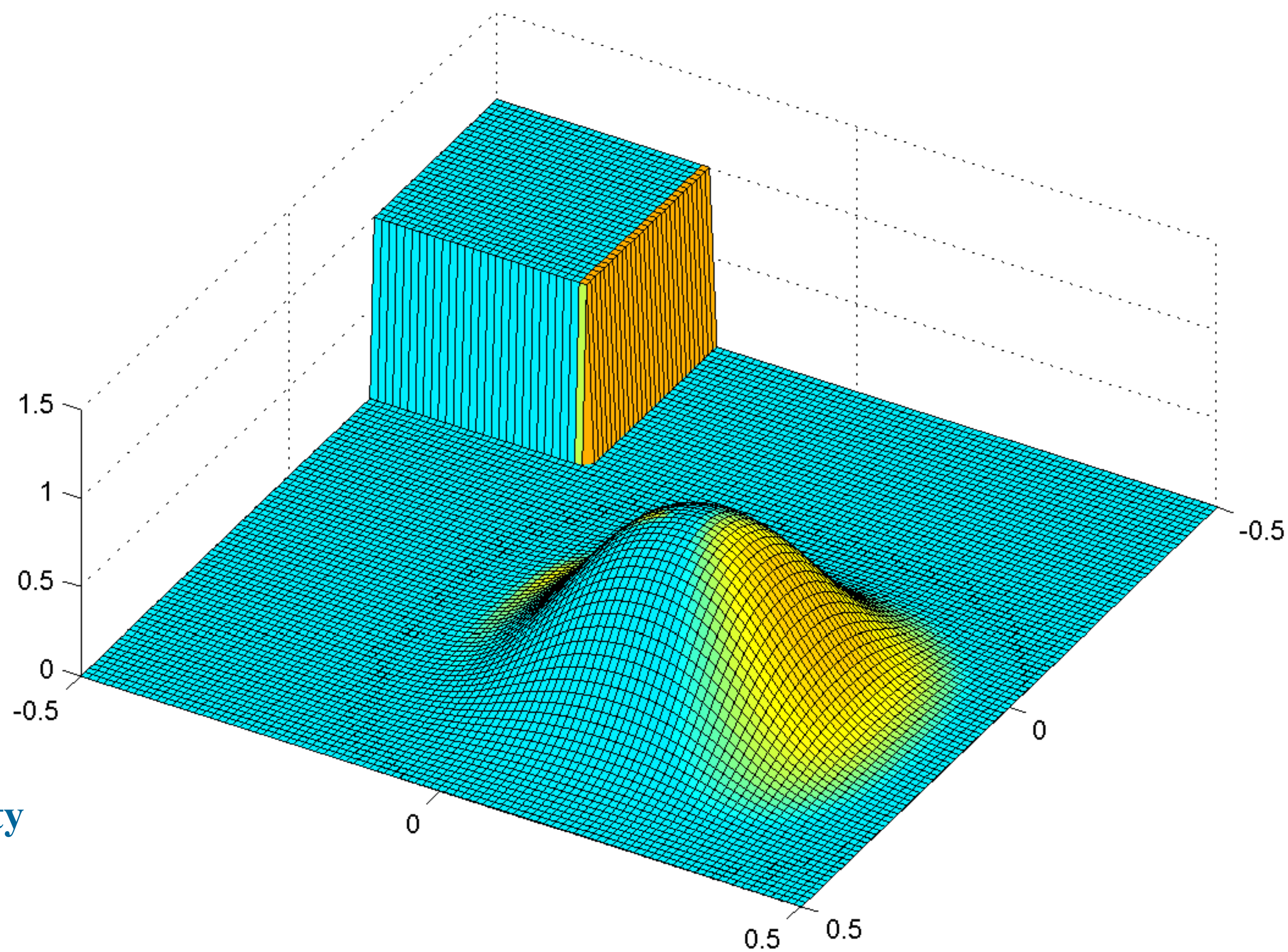


FEM from the left side CN in time, full implicit in time, with up-winding

Finite-difference
No Upstream Weighting

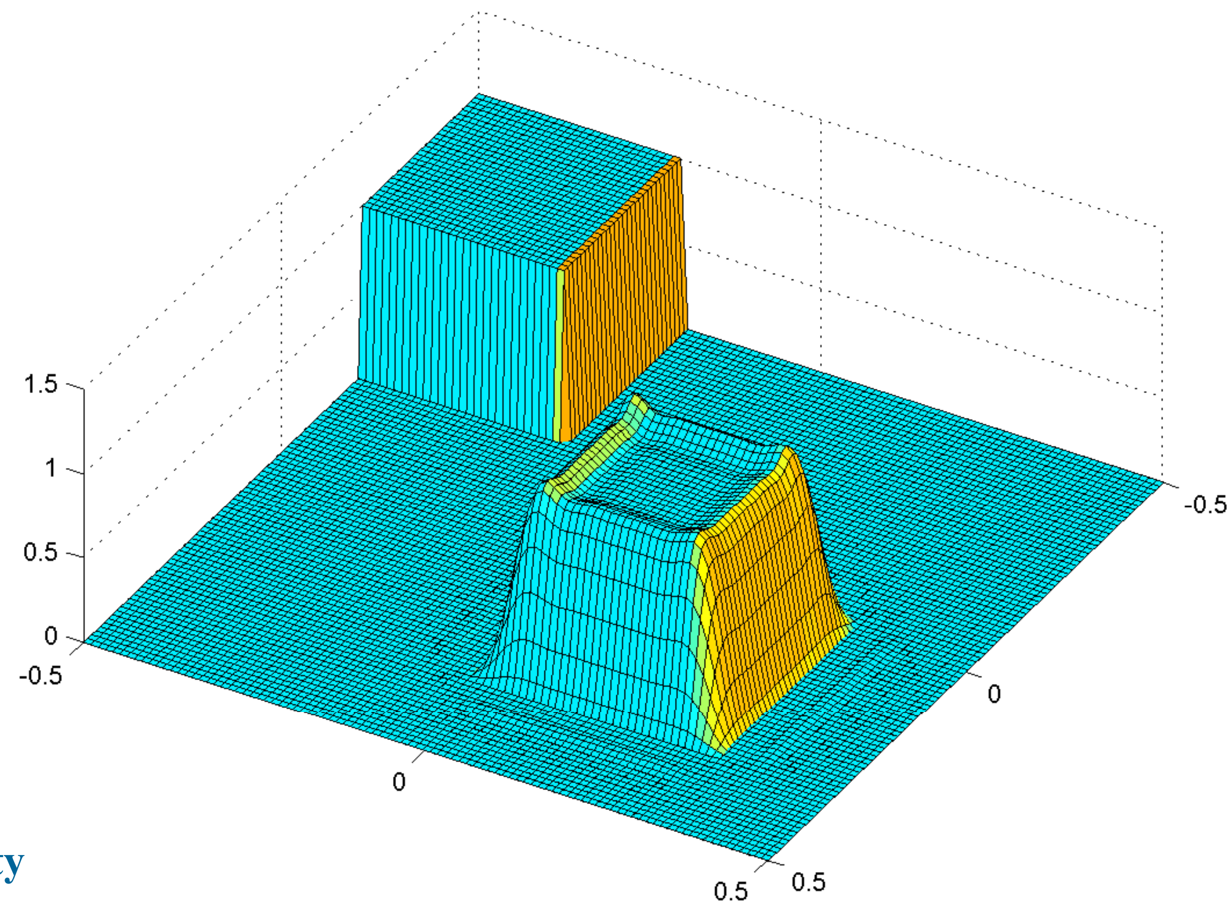


Translating Tower
Finite-difference Method



Pe=Infinity
C_{ou}=0.32

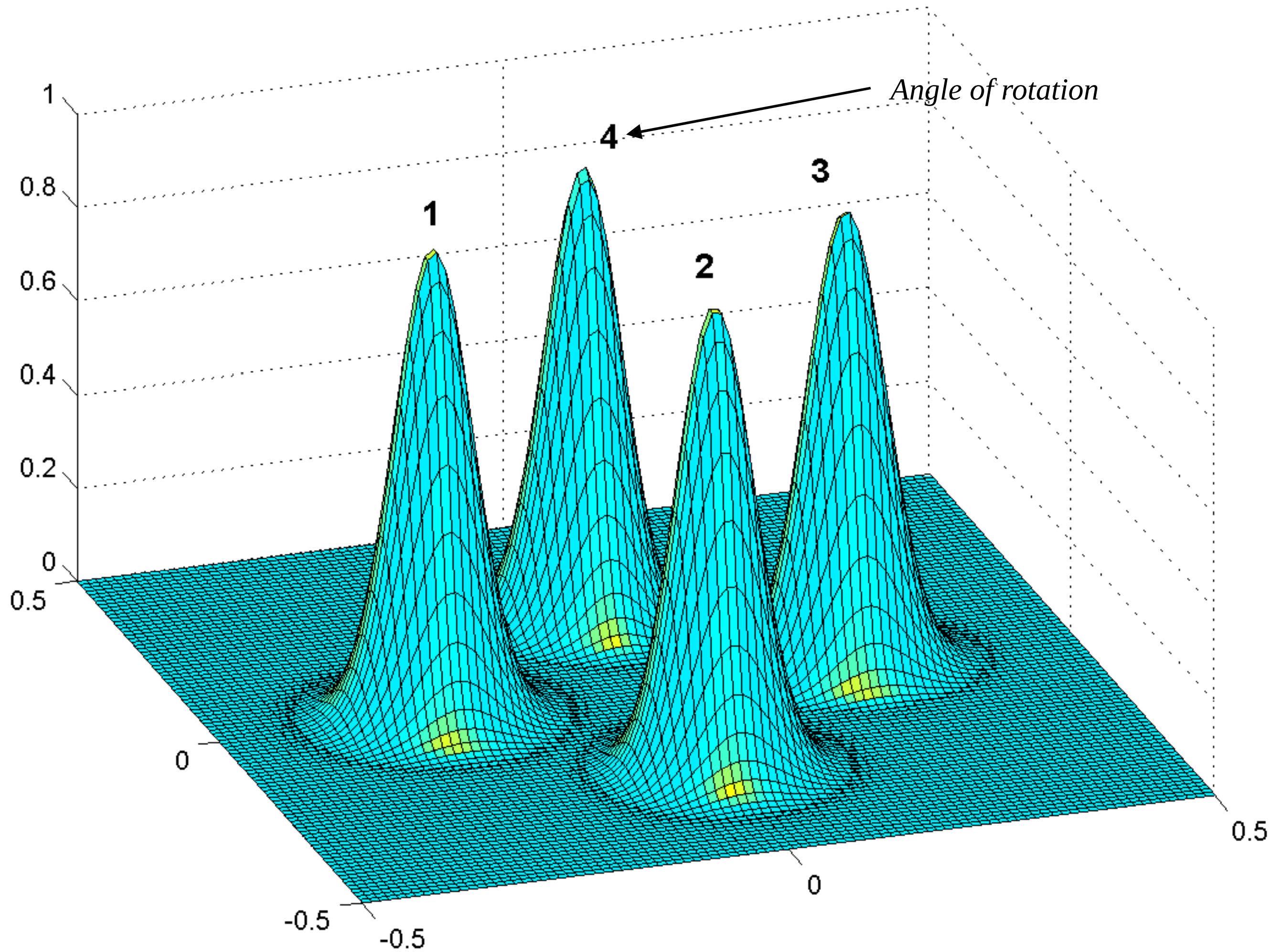
Translating Tower
LOCOM



Pe=Infinity

c_{ou}=0.32

Rotating Gauss Hill



ACCURACY OF A NUMERICAL SCHEME

Order of convergence in sup-norm

Valid for initial smooth conditions

for sharp front initial condition

*higher order schemes give "**oscillatory behavior**"*

*lower order schemes (up-wind) "**may work better**"*

WHY ???

IMPULSE RESPONSE - SOLUTION

Analytical solution for initial condition $u_n(t=0)=\delta_{0,n} \quad \forall n \in Z$

$$a_1 \frac{du_{i-1}}{dt} + a_2 \frac{du_i}{dt} + a_3 \frac{du_{i+1}}{dt} + b_1 u_{i-1} + b_2 u_i + b_3 u_{i+1} = 0 \qquad \forall i = 1,2,..,N_X$$

$$G(z,t) = \sum_{n=-\infty}^{\infty} u_n(t) z^n$$ **Generating function**

If G analytic ⟹ $$u_n(t) = \frac{1}{2\pi i} \oint_{\Gamma} G(z,t)\ z^{-n}\, dz$$

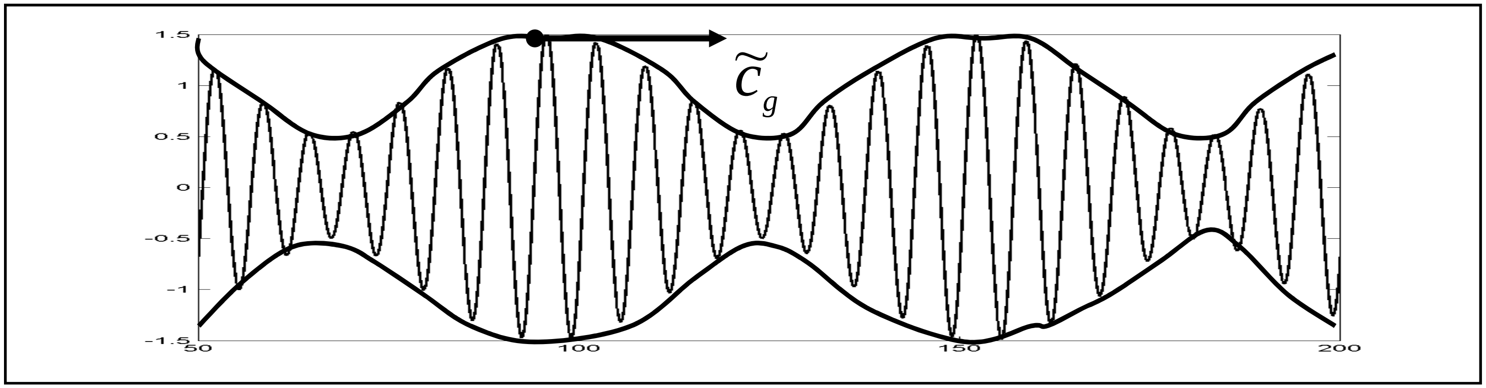
$$G(z,t) = \exp\left[-\frac{b_1 z^2 + b_2 z + b_3}{a_1 z^2 + a_2 z + a_3} t \right]$$

IMPULSE RESPONSE - GROUP VELOCITY

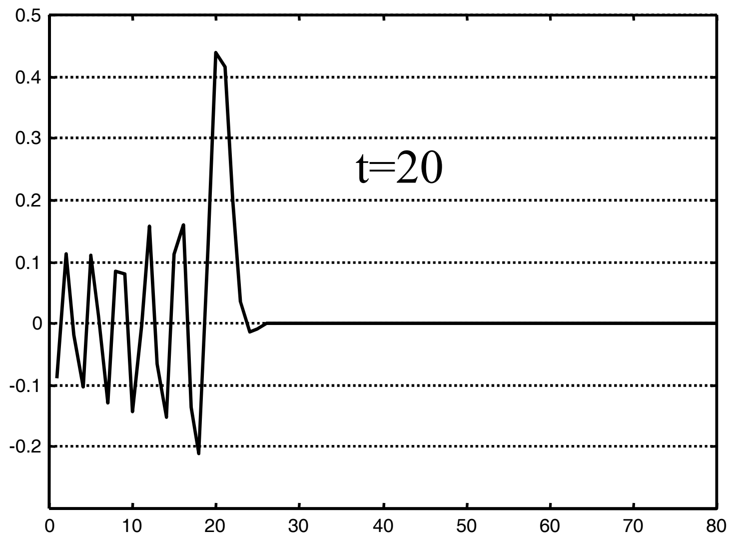
$$u_n(t) = \frac{1}{\pi}\int_0^{\pi} e^{-R(\omega)t}\cos[P(\omega)t - n\omega]\,d\omega$$

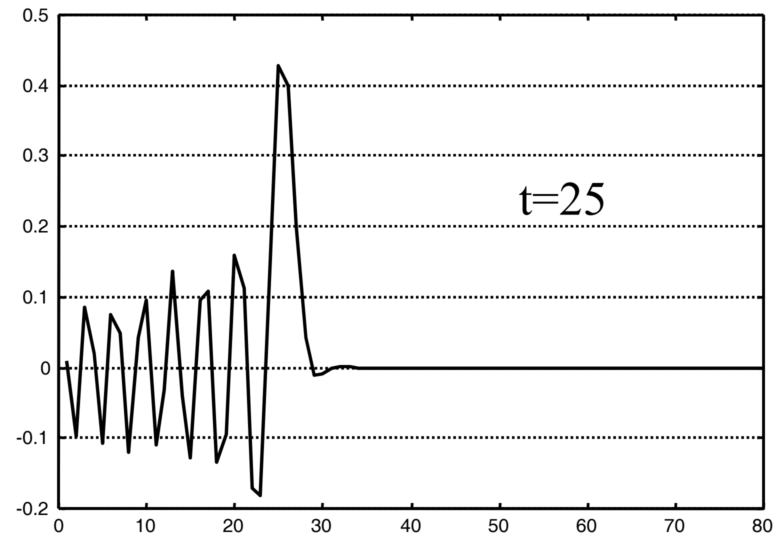
$$\tilde{c}_g = \frac{dP}{d\omega}$$ **Group velocity**

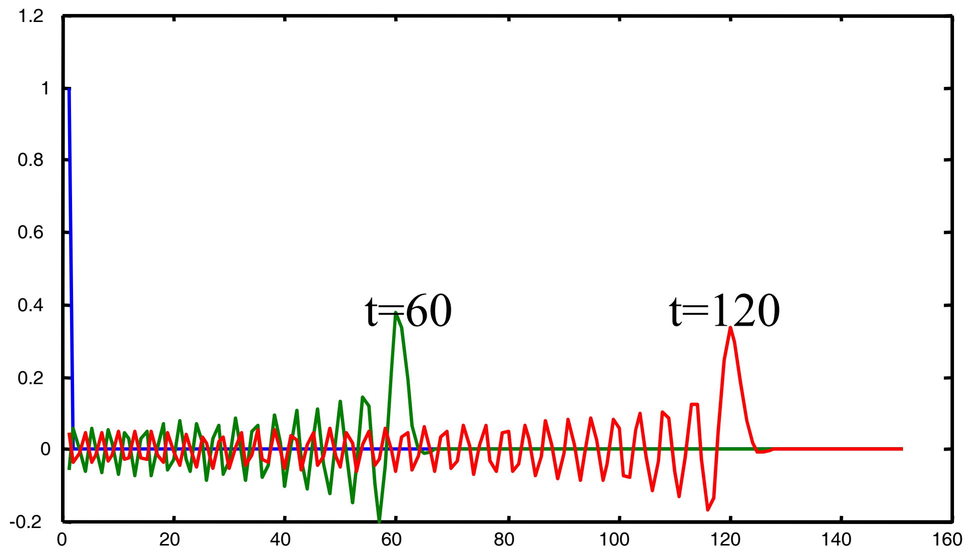
Wave envelope



IMPULSE RESPONSE - FEM

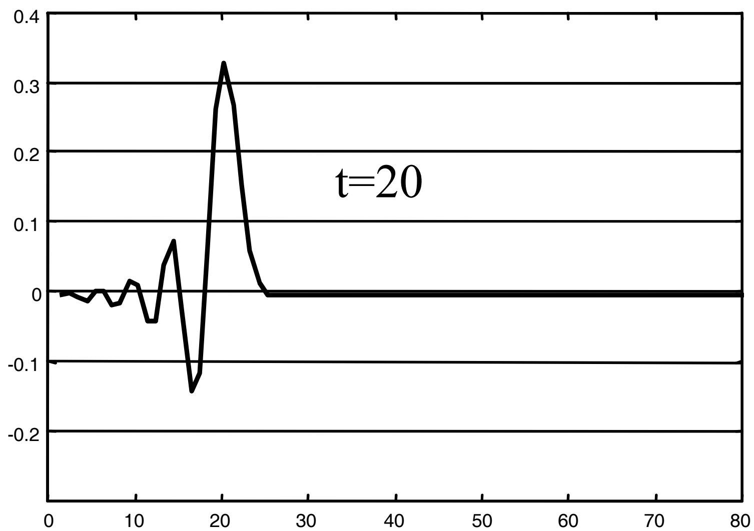


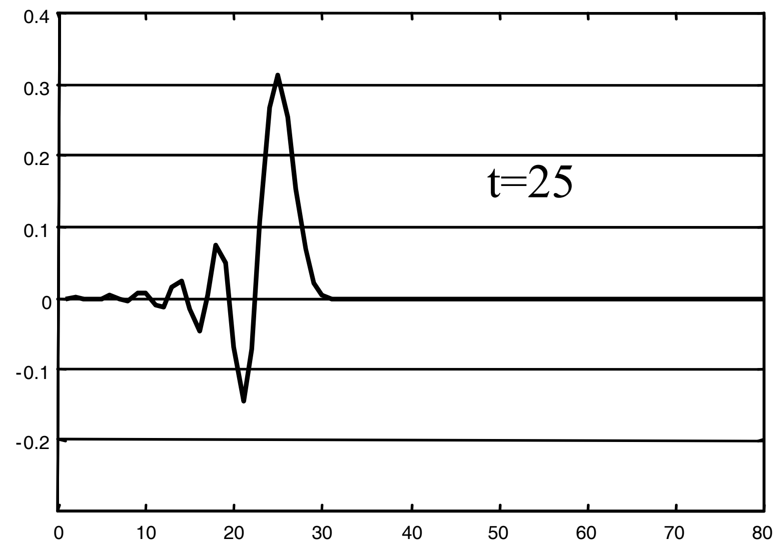




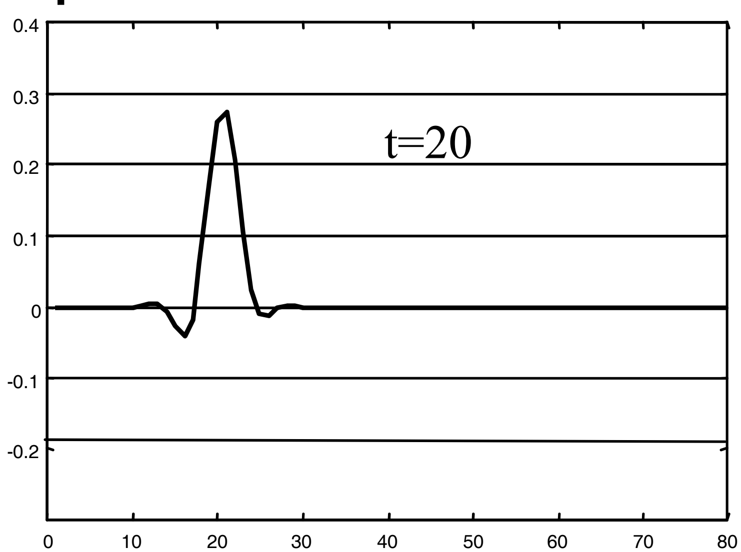
IMPULSE RESPONSE - LOCOM

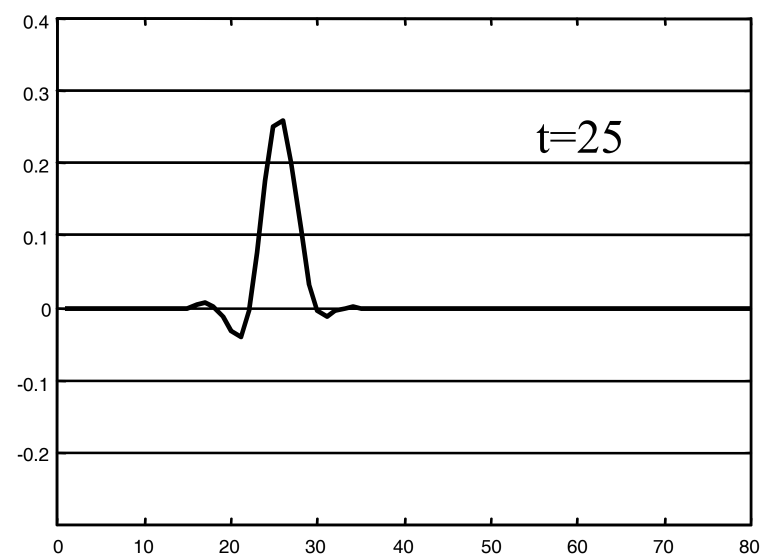
Partial up-wind

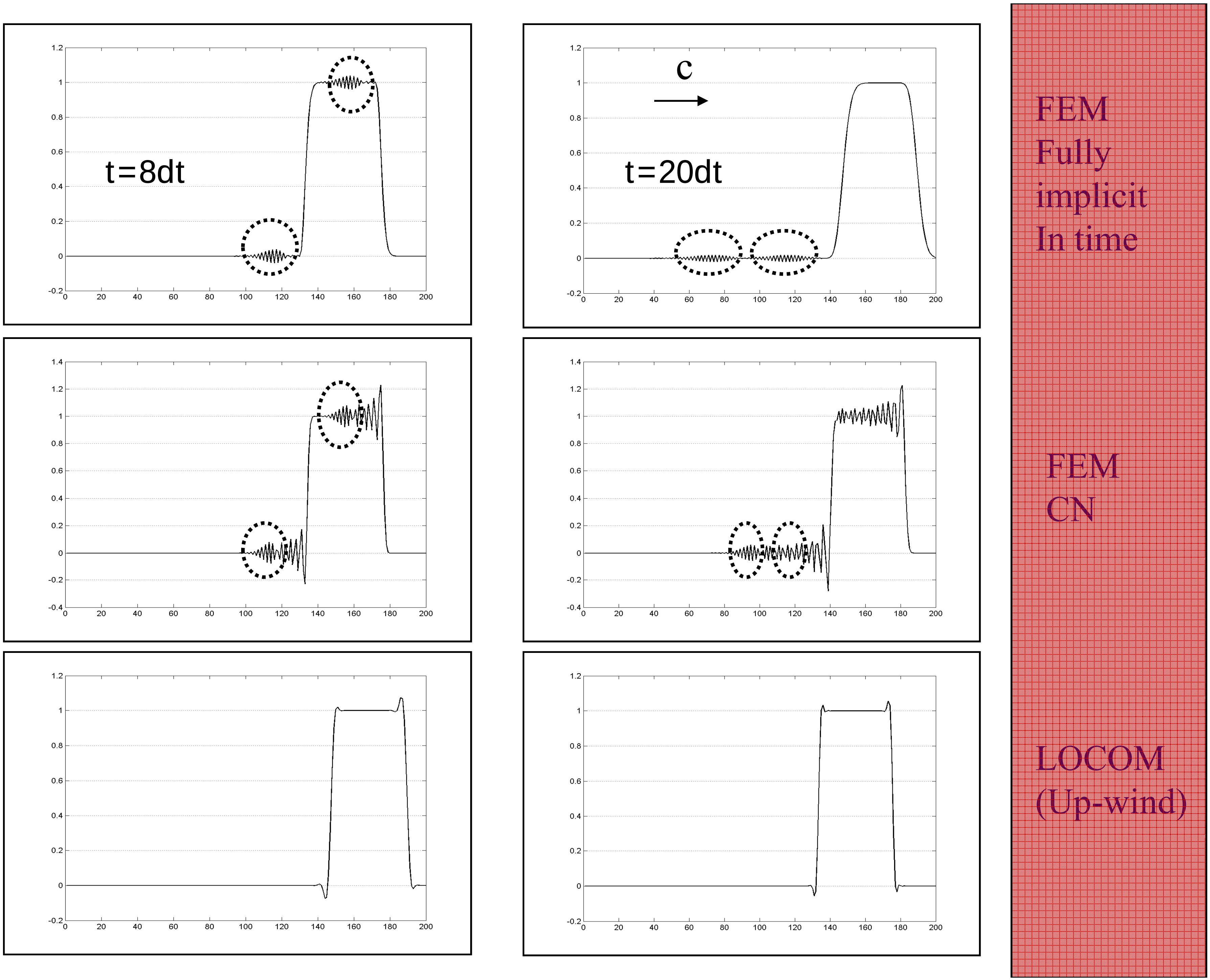




Full up-wind

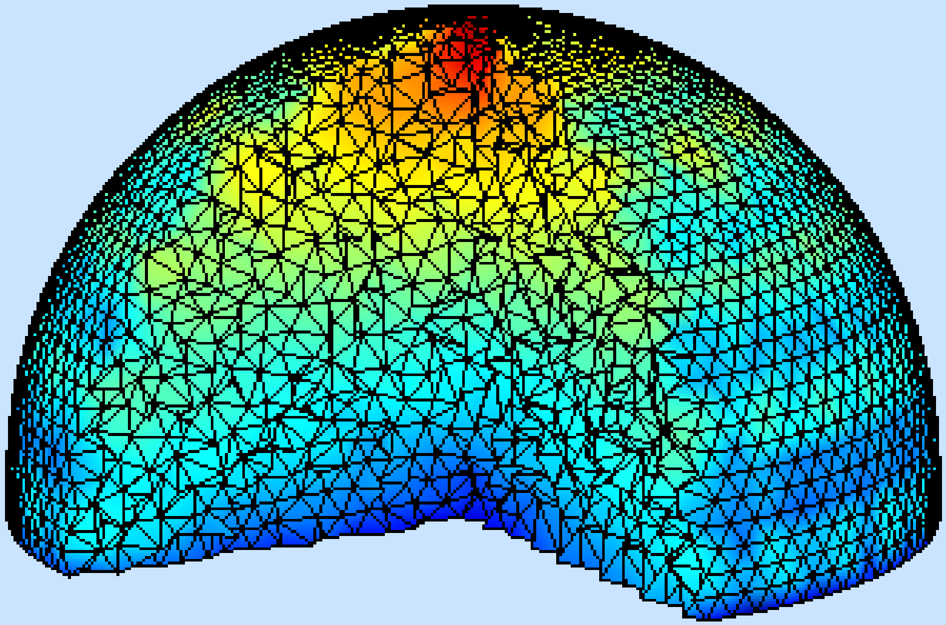





t=8dt
t=20dt
c
FEM
Fully
implicit
In time
FEM
CN
LOCOM
(Up-wind)

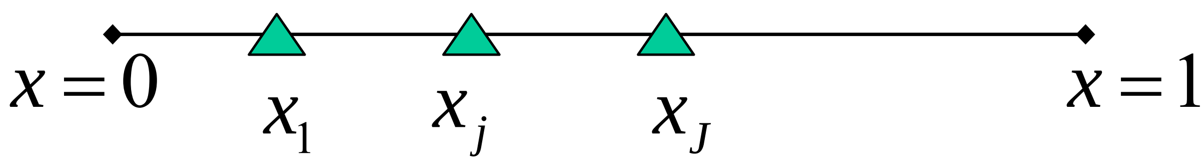
ADJOINT METHODS

FOR FLUORESCENCE TOMOGRAPHY



$$\frac{d^2u}{dx^2} + k(x)u = f(x) \qquad u(0) = 0, \quad u(1) = 0$$

$$k(x) = \sum_{n=1}^{N} K_n \psi_n(x) \qquad \{K_n\}_{n=1,\ldots N}$$



$$u(x_j) = \hat{u}_j, \qquad j = 1,\ldots J$$ **J Measurements**

find $\{\hat{K}_n\}$ such that $\min\limits_{\{K_n\}} \sum_{j=1}^{J} \left[u(x_j) - \hat{u}_j\right]^2$

$$2\sum_{j=1}^{J} \left[u(x_j) - \hat{u}_j\right] \left(\frac{\delta u(x_j)}{\delta K_n}\right) = 0$$

$$\frac{\delta u(x_j)}{\delta K_n} \ ?$$

$$\frac{d^2u}{dx^2} + ku = f(x) \qquad u(0) = 0, \quad u(1) = 0$$

$$k \rightarrow k + \delta k \qquad u \rightarrow u + \delta u \qquad \delta k = \delta K_n \psi_n(x)$$

$$\frac{d^2u}{dx^2} + \frac{d^2\delta u}{dx^2} + (k + \delta k)(u + \delta u) = f(x) \qquad u(0) + \delta u(0) = 0, \quad u(1) + \delta u(1) = 0$$

Perturbation equation

$$\frac{d^2\delta u}{dx^2} + k\delta u = -\delta k\, u(x) \qquad \delta u(0) = 0, \ \ \delta u(1) = 0$$

Perturbation equation

$$\frac{d^2\delta u}{dx^2} + k\delta u = -\delta K_n \psi_n(x) u(x) \qquad \delta u(0) = 0,\ \delta u(1) = 0$$

Green's function $$\frac{d^2 G}{dx^2} + kG = \delta(x - x_j) \qquad G(0) = 0,\ G(1) = 0$$

$$\int_0^1 G\left(\frac{d^2\delta u}{dx^2} + k\delta u\right)dx = -\delta K_n \int_0^1 G\psi_n(x) u(x) dx$$

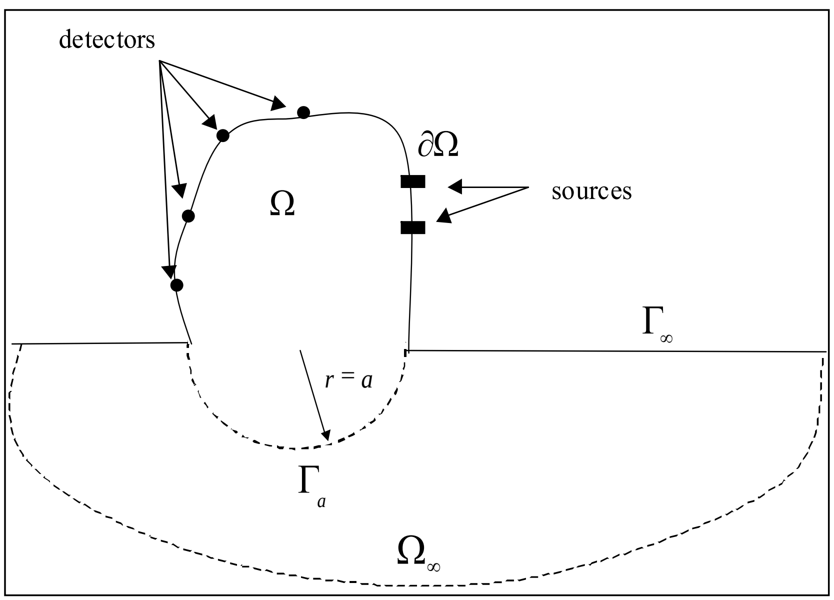
$$\int_0^1 \left(\frac{d^2 G}{dx^2} + kG\right)\delta u + \left[\frac{d\delta u}{dx} G - \frac{dG}{dx}\delta u\right]_0^1 = -\delta K_n \int_0^1 G\psi_n(x) u(x) dx$$

$$\delta u(x_j) = -\delta K_n \int_0^1 G(x - x_j)\psi_n(x) u(x) dx$$

Direct approach : N computations **Adjoint method: J computations**

FREQUENCY-DOMAIN PHOTON MIGRATION PDE's

$$
\begin{cases}
-\nabla \bullet \left(D_x \nabla \Phi_x \right) + k_x \Phi_x = S \\
-\nabla \bullet \left(D_m \nabla \Phi_m \right) + k_m \Phi_m = \beta \Phi_x
\end{cases}
\qquad
\begin{cases}
D_x \dfrac{\partial \Phi_x}{\partial n} + r_x \Phi_x = 0 \\
D_m \dfrac{\partial \Phi_m}{\partial n} + r_m \Phi_m = 0
\end{cases}
\quad on \quad \partial\Omega
$$



$$
\begin{cases}
-\underline{\underline{\nabla}}^t \left(\underline{\underline{\mathbf{d}}} \, \underline{\underline{\nabla}} \, \underline{\mathbf{\Phi}} \right) + \underline{\underline{\mathbf{k}}} \, \underline{\mathbf{\Phi}} = \underline{\mathbf{S}} \ \textbf{on} \quad \Omega \\
\underline{\underline{\mathbf{D}}} \dfrac{\partial \underline{\mathbf{\Phi}}}{\partial n} + \underline{\underline{\mathbf{r}}} \, \underline{\mathbf{\Phi}} = \underline{0} \quad \textbf{on} \quad \partial\Omega
\end{cases}
$$

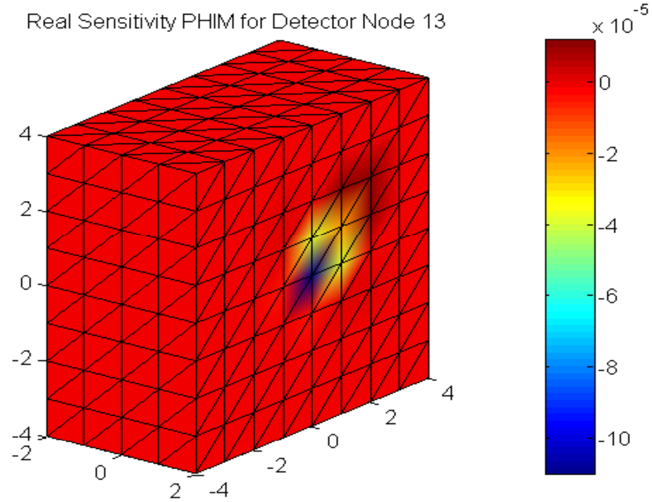
THE GREEN MATRIX

$$\underline{\delta\mathbf{\Phi}}(\underline{\mathbf{x}}_{\det}) = \int_{\Omega} \underline{\underline{\mathbf{\Psi}}}^{t}(\underline{\mathbf{x}};\underline{\mathbf{x}}_{\det})\left(\underline{\underline{\nabla}}^{t}\left(\frac{\partial \underline{\underline{\mathbf{d}}}}{\partial p}\delta p\,\underline{\underline{\nabla}}\,\underline{\mathbf{\Phi}}\right) - \frac{\partial \underline{\underline{\mathbf{k}}}}{\partial p}\delta p\,\underline{\mathbf{\Phi}}\right) d\Omega + \int_{\partial\Omega} \underline{\underline{\mathbf{\Psi}}}^{t}(\underline{\mathbf{x}};\underline{\mathbf{x}}_{\det})\left(-\frac{\partial \underline{\underline{\mathbf{D}}}}{\partial p}\delta p\,\frac{\partial \underline{\mathbf{\Phi}}}{\partial n} - \frac{\partial \underline{\underline{\mathbf{r}}}}{\partial p}\delta p\,\underline{\mathbf{\Phi}}\right) dS$$

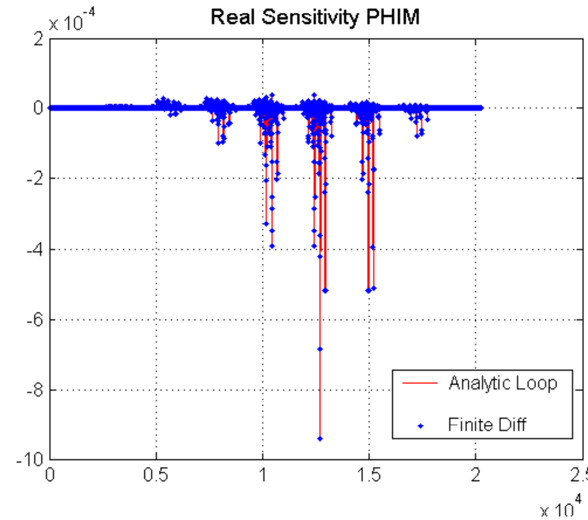
$$\underline{\underline{\mathbf{\Psi}}}(\underline{\mathbf{x}};\underline{\mathbf{x}}_{\det}) = \begin{bmatrix} \mathbf{\Psi}_{xx}(\underline{\mathbf{x}};\underline{\mathbf{x}}_{\det}) & \mathbf{\Psi}_{xm}(\underline{\mathbf{x}};\underline{\mathbf{x}}_{\det}) \\ \mathbf{\Psi}_{mx}(\underline{\mathbf{x}};\underline{\mathbf{x}}_{\det}) & \mathbf{\Psi}_{mm}(\underline{\mathbf{x}};\underline{\mathbf{x}}_{\det}) \end{bmatrix} \Longrightarrow \begin{cases} -\underline{\underline{\nabla}}^{t}\left(\underline{\underline{\mathbf{d}}}\,\underline{\underline{\nabla}}\,\underline{\underline{\mathbf{\Psi}}}\right) + \underline{\underline{\mathbf{k}}}^{t}\,\underline{\underline{\mathbf{\Psi}}} = \underline{\underline{\mathbf{\delta}}}(\underline{\mathbf{x}};\underline{\mathbf{x}}_{\det}) \text{ on } \Omega \\ \underline{\underline{\mathbf{D}}}\frac{\partial \mathbf{\Psi}}{\partial n} + \underline{\underline{\mathbf{r}}}\,\underline{\underline{\mathbf{\Psi}}} = 0 \text{ on } \partial\Omega. \end{cases}$$

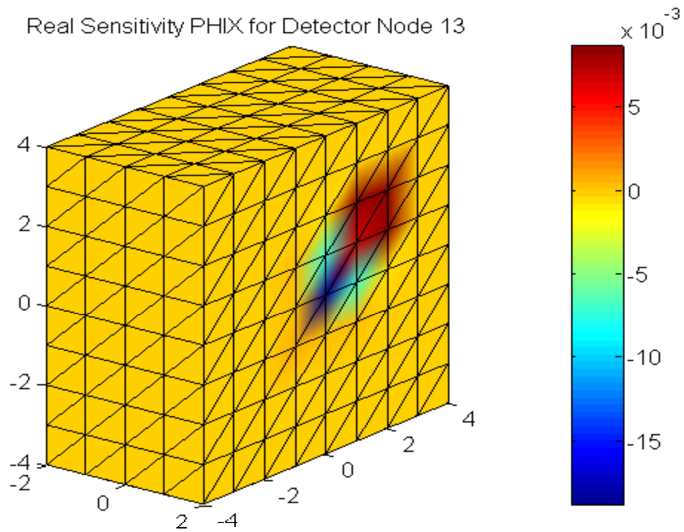
Sample Results: small homogeneous domain

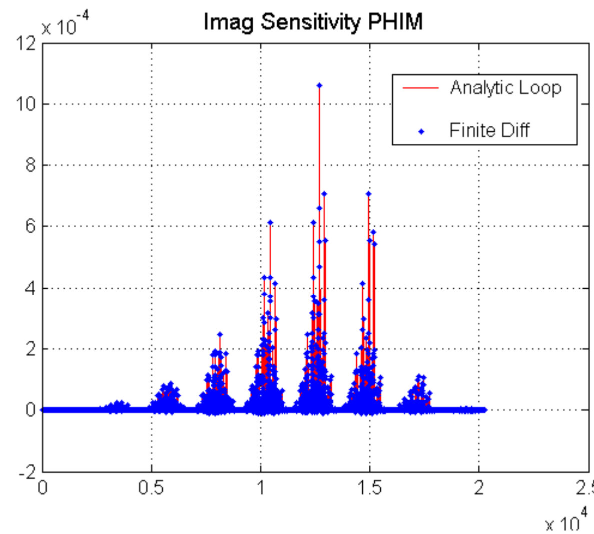
(405 nodes, 1536 elements, 1 source, 50 detectors)



$$\frac{\partial \Phi_m}{\partial \mu_{axf}}$$





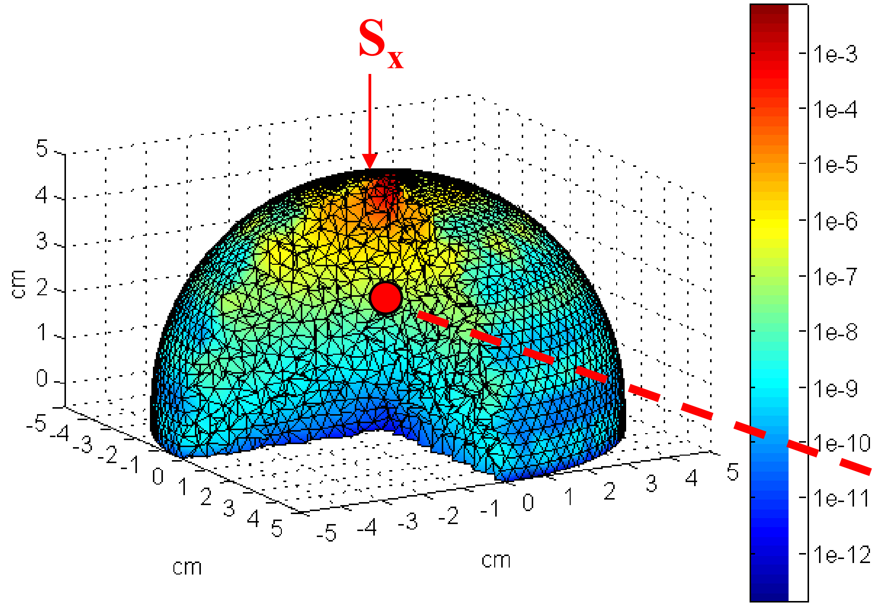


Run time (850 Mhz Pentium III)
Adjoint 0.23 min
FD 4.07 min

Adjoint and FD results were identical.

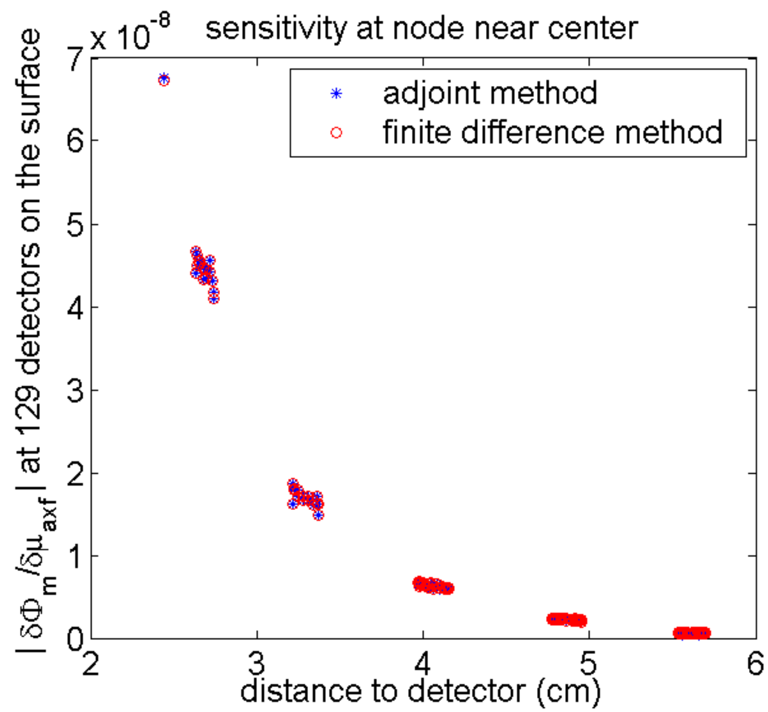
Sample Results: large (breast-shaped) homogeneous domain

(12657 nodes, 65509 elements, 1 source, 129 detectors)



$$\frac{\partial \Phi_m}{\partial \mu_{axf}}$$ Adjoint: 19 min

FD: projected 9 days

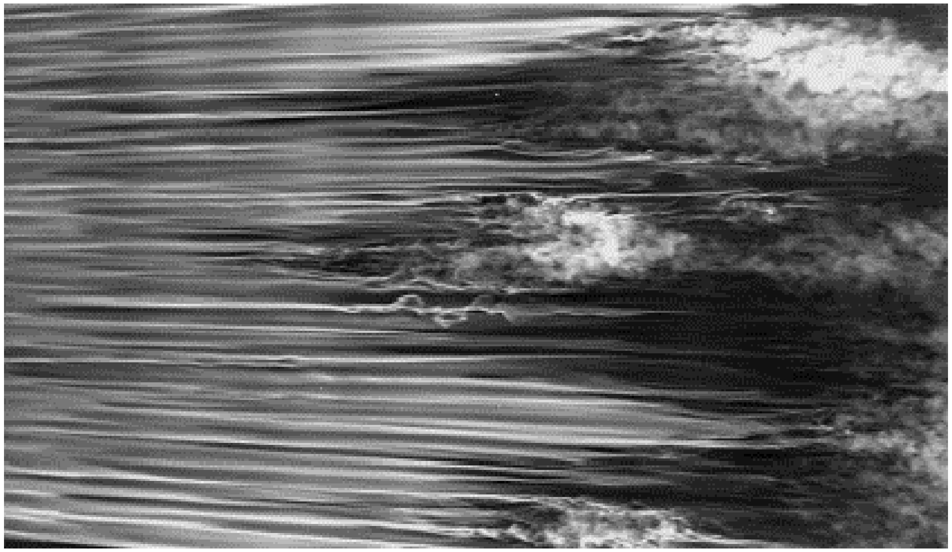


Sensitivity drops off exponentially with distance to detector.

Adjoint and FD within 1e-9 of each other.

REVISITING THE STABILITY OF

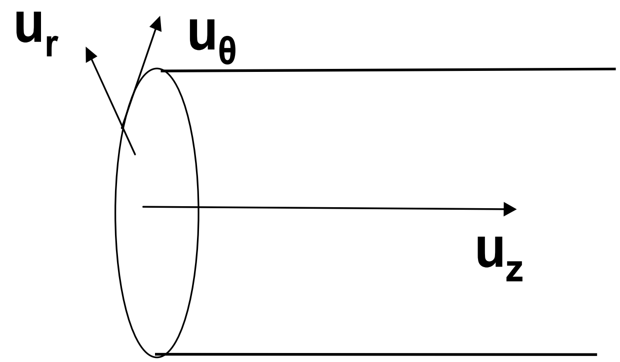
PULSATILE PIPE FLOW



Womersley* solution for pulsatile pipe flow

$$\frac{\partial W}{\partial t} - \nu \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial W}{\partial r}\right) = -\frac{1}{\rho}\frac{\partial P}{\partial z}$$

$$\frac{\partial P}{\partial z} = -\left[K_0 + K_\omega \exp(i\omega t)\right]$$

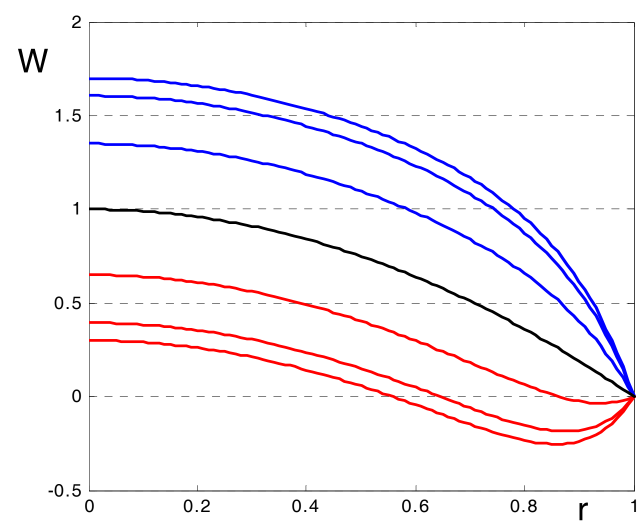


$$W(r,t) = \frac{K_0}{4\mu}(R^2 - r^2) + \frac{R^2}{i\mu \mathrm{Wo}}\left[1 - \frac{J_0\left(i^{3/2}\mathrm{Wo}\frac{r}{R}\right)}{\left(i^{3/2}\mathrm{Wo}\right)}\right]K_\omega \exp(i\omega t)$$

- The flow is linearly stable for axisymmetric perturbations (Tozzi & von Kerczek, 1986)

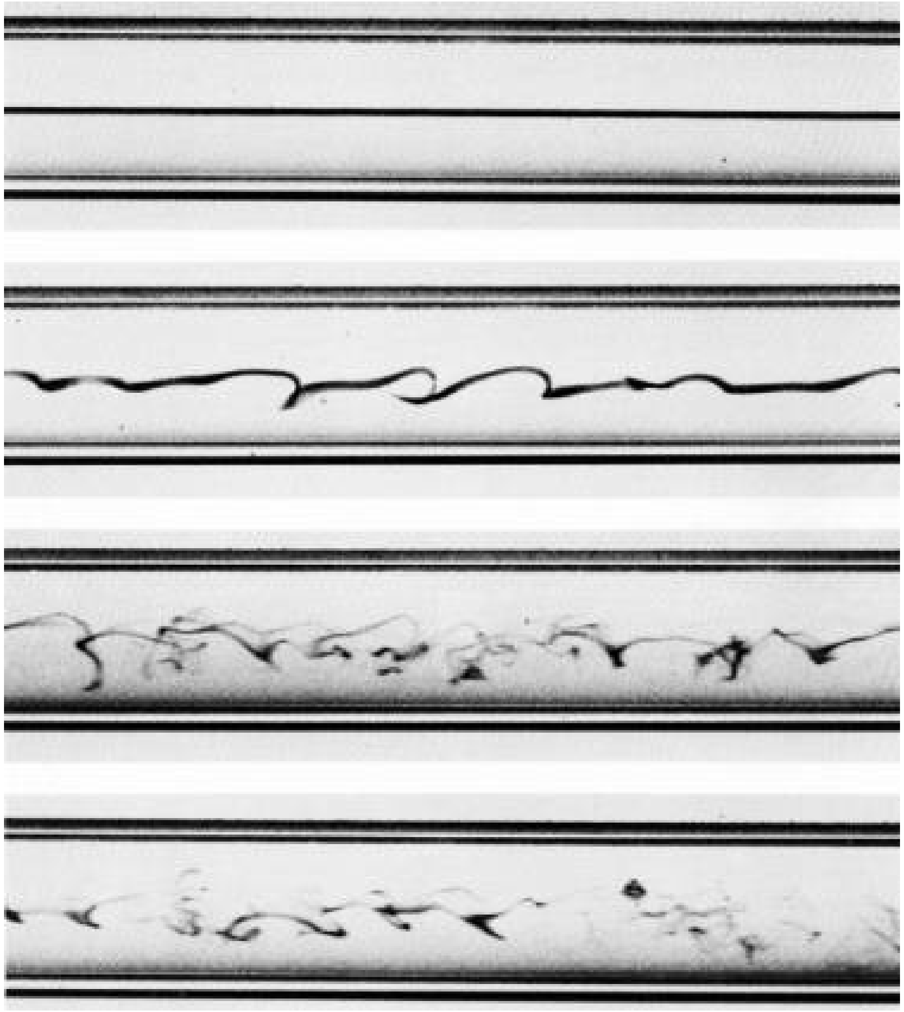
- Slightly more stable than Poiseiulle flow

- Presence of inflection rings occur during an oscillation cycle for “sufficiently strong” flow pulsation in relation to the mean flow



* Womersley J.R., Method for the Calculation of Velocity, Rate of Flow and Viscous Drag in Arteries When the Pressure Gradient is Known. J. Physiol., 127 (1955), pp. 553-563.

Reynolds pipe flow experiment

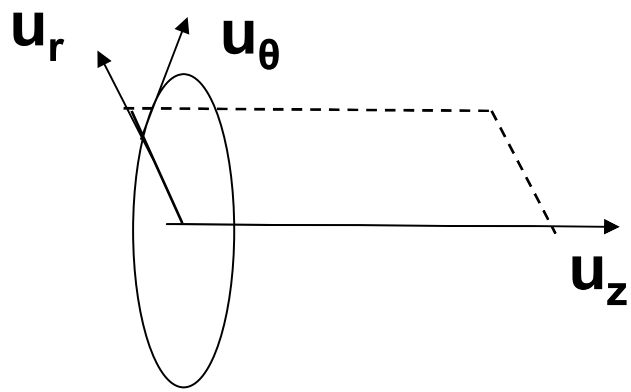


The Orr-Sommerfeld Equation

Linear stability analysis; axisymmetric perturbations

$$u_r = u \qquad u_\theta = 0 \qquad u_z = W + w$$

Stokes Stream function



$$u = -\frac{\psi}{r} i\alpha \exp(i\alpha z) \qquad w = \frac{1}{r}\frac{\partial \psi}{\partial r}\exp(i\alpha z)$$

Result: Orr-Sommerfeld Equation…

$$\frac{\partial (L\psi)}{\partial t} - Wi\alpha^3\psi + i\alpha(-\psi LW + W L\psi) = \mathrm{Re}^{-1} L^2\psi$$

$$\frac{\psi}{r} < \infty \qquad \frac{1}{r}\frac{\partial \psi}{\partial r} < \infty \qquad as \qquad r \to 0^+$$

$$\psi(1,t) = \frac{\partial \psi}{\partial r}(1,t) = 0$$

$$\mathrm{L}\psi = \frac{\partial^2 \psi}{\partial r^2} - \frac{1}{r}\frac{\partial \psi}{\partial r} - \alpha^2$$

Long-wave Orr-Sommerfeld basis

Longwave limit of the Orr Sommerfeld equation:

$$\frac{\partial\left(\widetilde{L}\,\psi\right)}{\partial t} = \mathrm{Re}^{-1}\,\widetilde{L}^2\psi$$

$$\widetilde{\mathrm{L}}\psi = \frac{\partial^2\psi}{\partial r^2} - \frac{1}{r}\frac{\partial\psi}{\partial r}$$

Analytical solution in longwave limit

$$\psi(r,t) = \sum_{n=1}^{\infty} a_n \phi_n(r) \exp(-\lambda_n t)$$

$$\phi_n(r) = \frac{\sqrt{2}}{4\chi_n} r\left(1 - \frac{J_1(\chi_n r)}{J_1(\chi_n)}\right)$$

Orthogonal with respect to the Scalar product

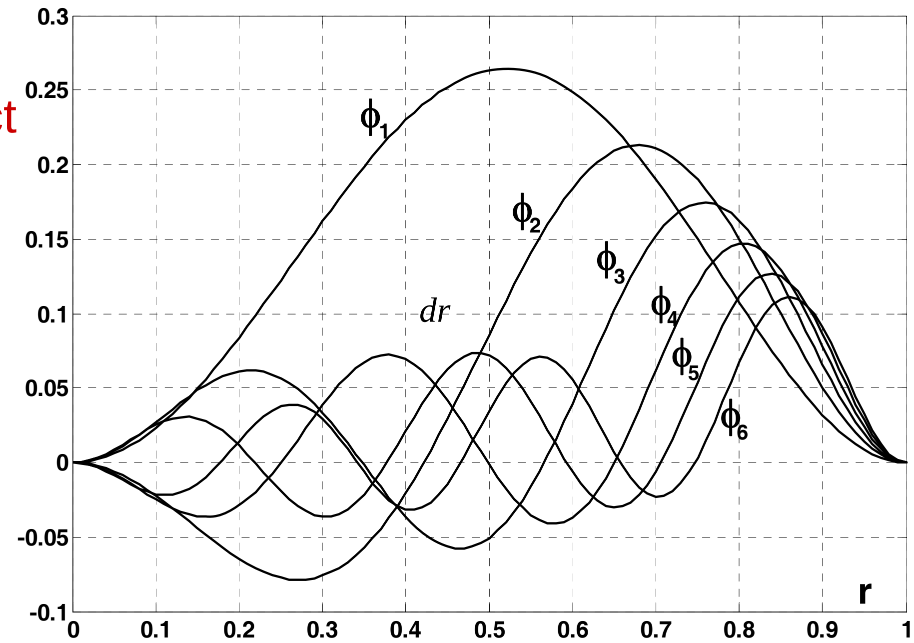
$$\langle f, g\rangle = \int_0^1 \frac{\partial f}{\partial r}\frac{\partial g}{\partial r}\frac{dr}{r}$$

☺

Non orthogonal with respect to

$$\langle f, g\rangle = \int_0^1 f\, g\, dr$$

☹



Galerkin Method

$$\hat{\psi}(r,t) = \sum_{n=1}^{\infty} a_n(t)\phi_n(r)$$

Boundary conditions satisfied a priori

Galerkin projection

$$\left\langle \frac{\partial(L\hat{\psi})}{\partial t} - Wi\alpha^3\hat{\psi} + i\alpha\left(-\hat{\psi}LW + W L\hat{\psi}\right) - \mathrm{Re}^{-1} L^2\hat{\psi}, \phi_n \right\rangle = 0$$

$$\frac{d\mathbf{a}}{dt} = \mathbf{M}^{-1}\left[\underbrace{\mathbf{K}}_{\text{steady flow}} + \underbrace{\mathbf{H}\exp\left(it\,\mathrm{St}\right)}_{\text{oscillation}}\right]\mathbf{a}$$

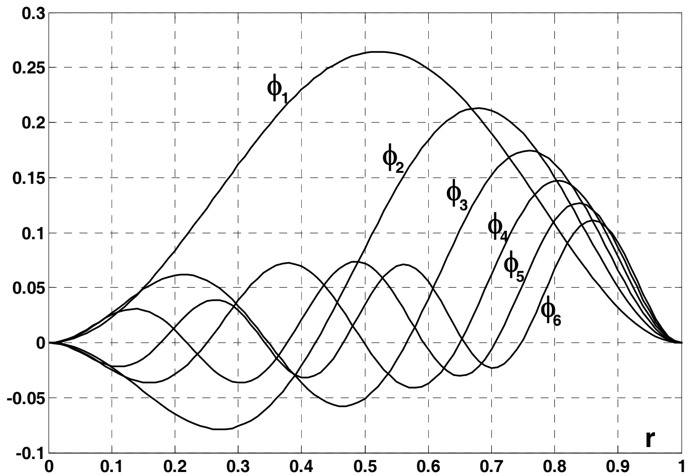
steady flow oscillation

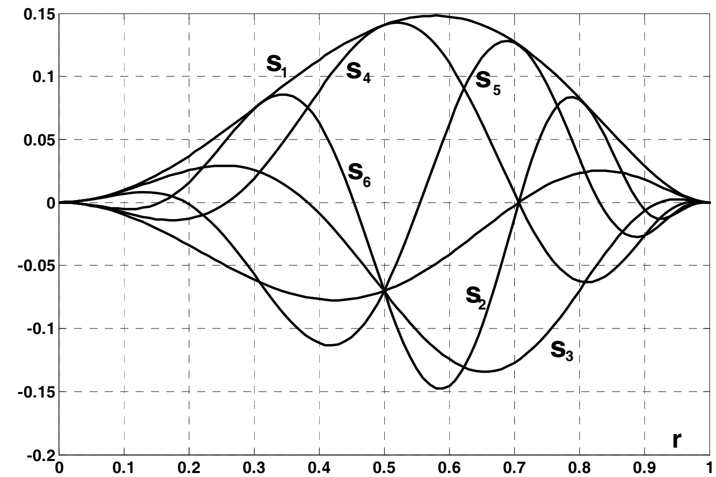
Energy of the perturbation $E(\mathbf{a},t) = \frac{1}{2}\mathbf{a}^*\mathbf{M}\mathbf{a}$

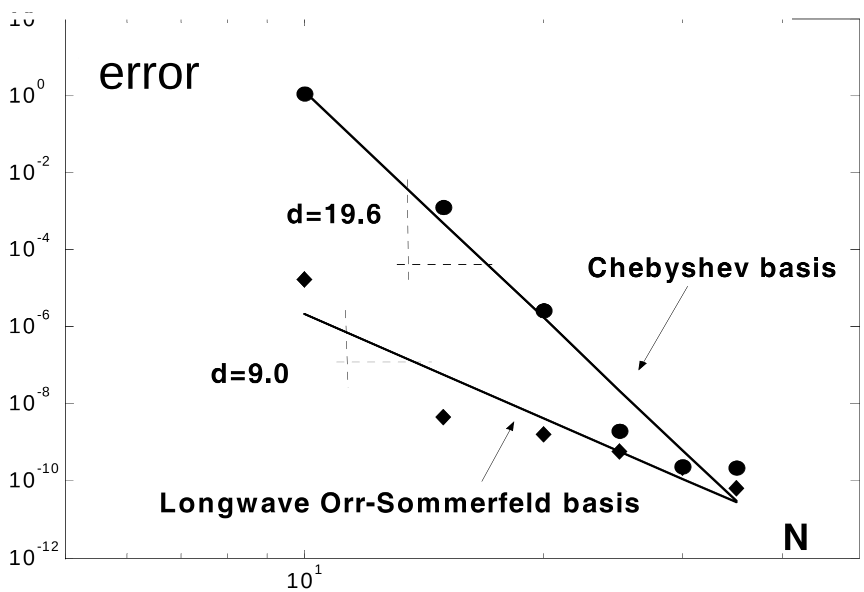
Convergence and accuracy

$$\phi_n(r) = \frac{\sqrt{2}}{4\chi_n} r \left(1 - \frac{J_1(\chi_n r)}{J_1(\chi_n)}\right)$$

$$s_n(r) = r^2(1-r^2)^2 T_{2n-2}(r)$$







$$\frac{d\mathbf{a}}{dt} = \mathbf{M}^{-1}\left[\mathbf{K} + \mathbf{H}\exp(it\,\mathrm{St})\right]\mathbf{a}$$

Steady flow case

First eigenvalue

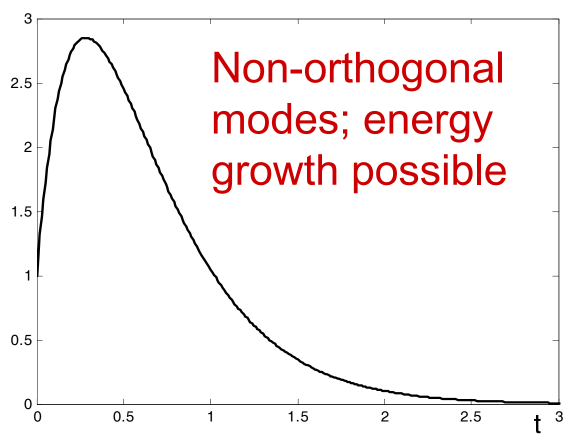
Transient energy growth

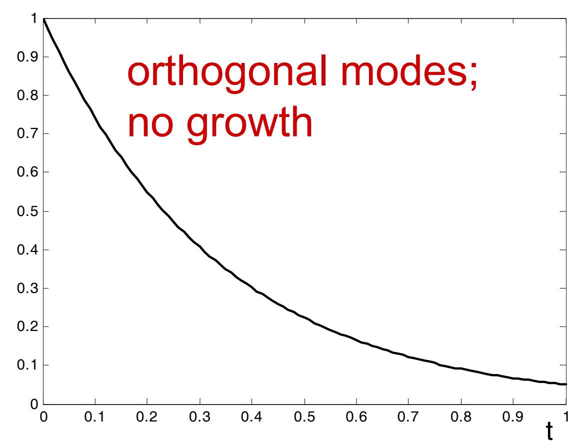
$$u(r,t)=\sum_{n=1}^{\infty} a_n \phi_n(r)\exp\left(-\lambda_n t\right)$$

Initial conditions

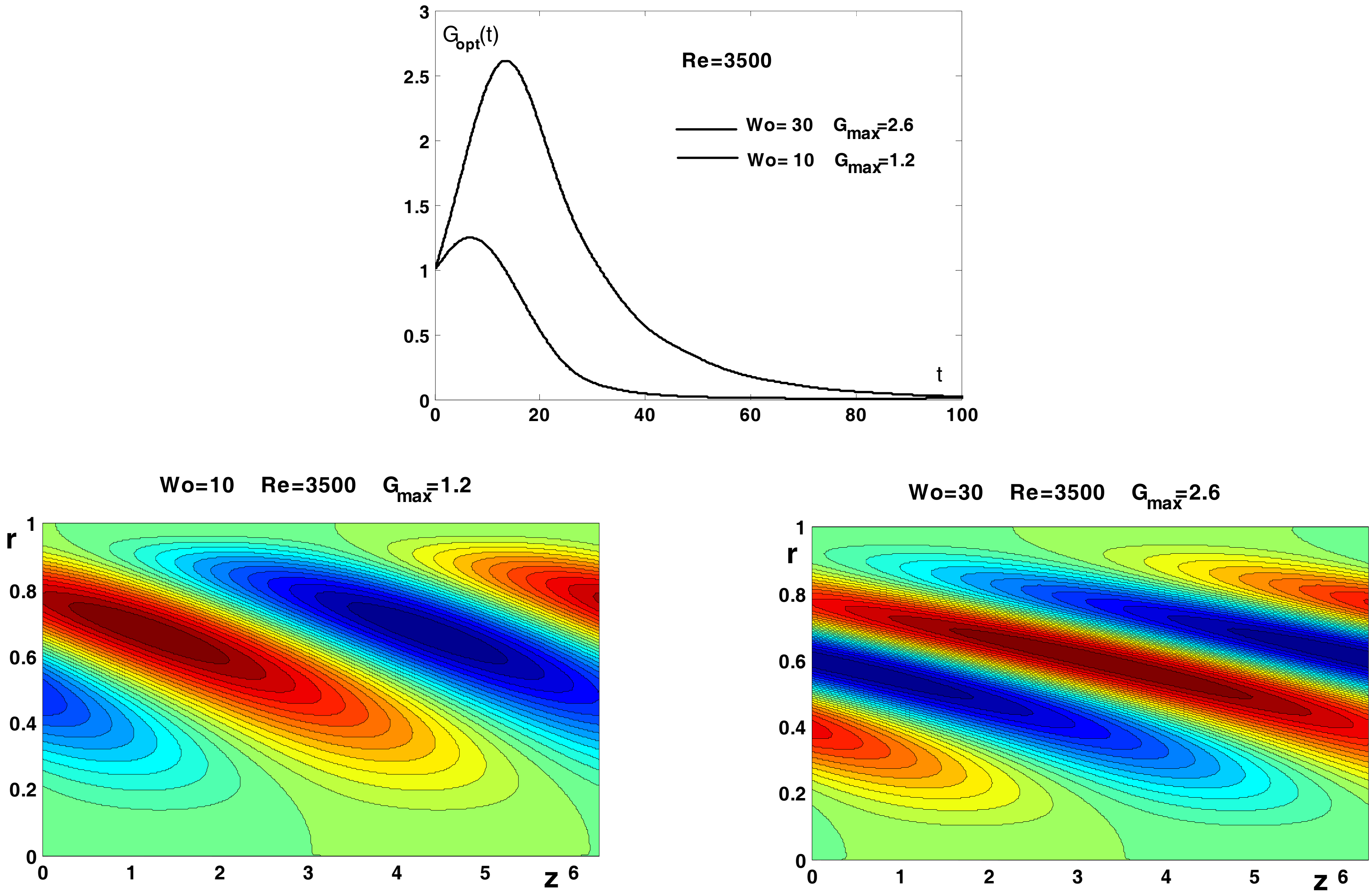
Set of non orthogonal eigenmodes $\langle \phi_n , \phi_m \rangle = \int_0^1 \phi_n \, \phi_m \, dr \neq \delta_{nm}$

$$E(r,t)=\int_0^1 u^* u dr = \sum_{n}^{\infty} a_n^* a_m^* \langle \phi_n(r)\phi_m(r)\rangle e^{-(\lambda_n+\lambda_m)t} \neq \sum_{n,m}^{\infty} |a_n|^2 e^{-2\lambda_n t}$$

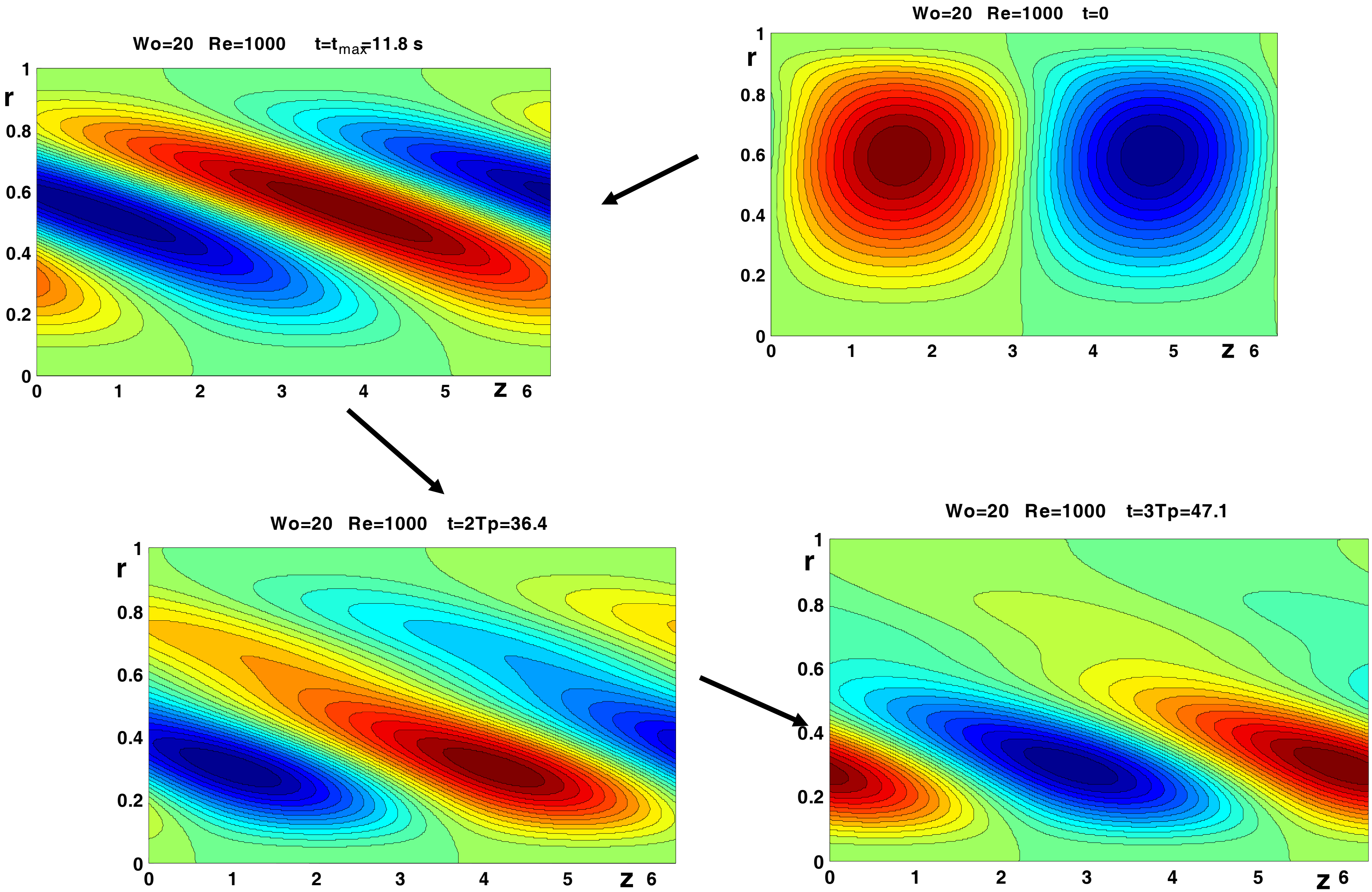




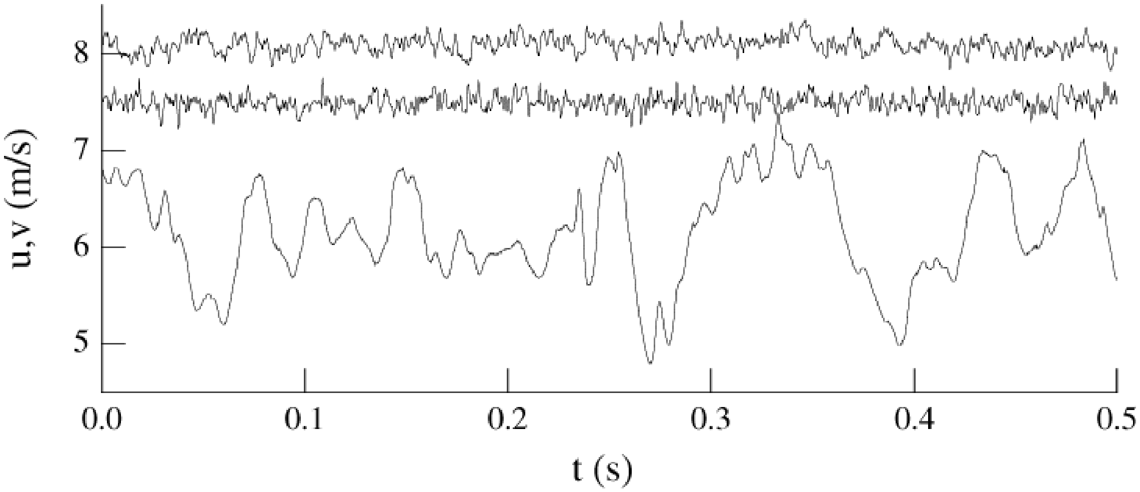
Optimal Perturbations : Maximum Energy Growth

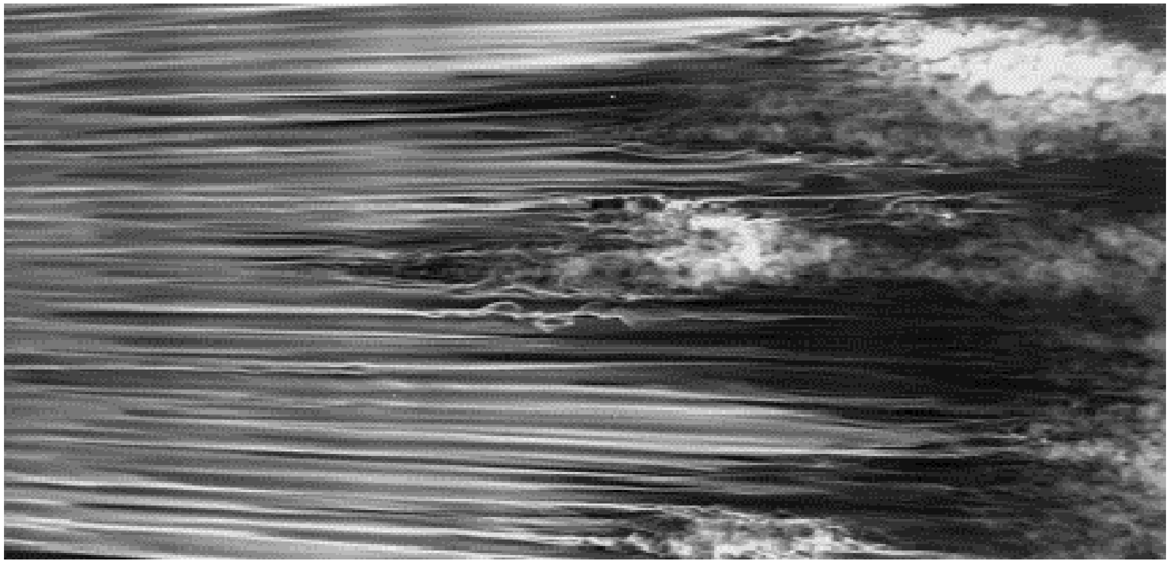


Time evolution optimal perturbation



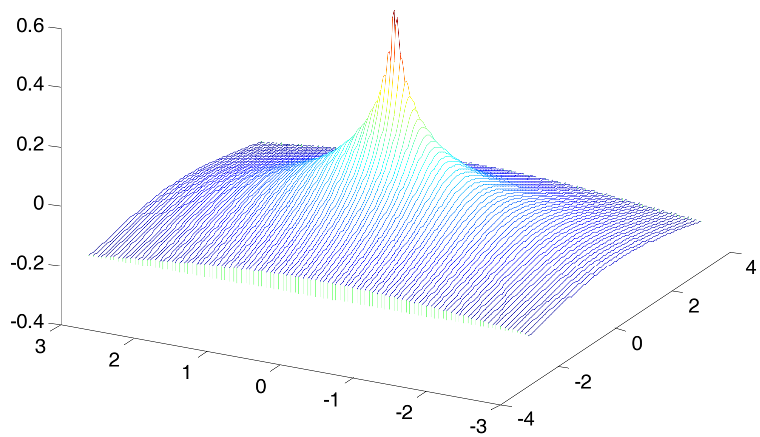
FREE-STREAM TURBULENCE AND STREAK BREAKDOWN





A BOUNDARY ELEMENT METHOD

FOR FLUORESCENCE TOMOGRAPHY

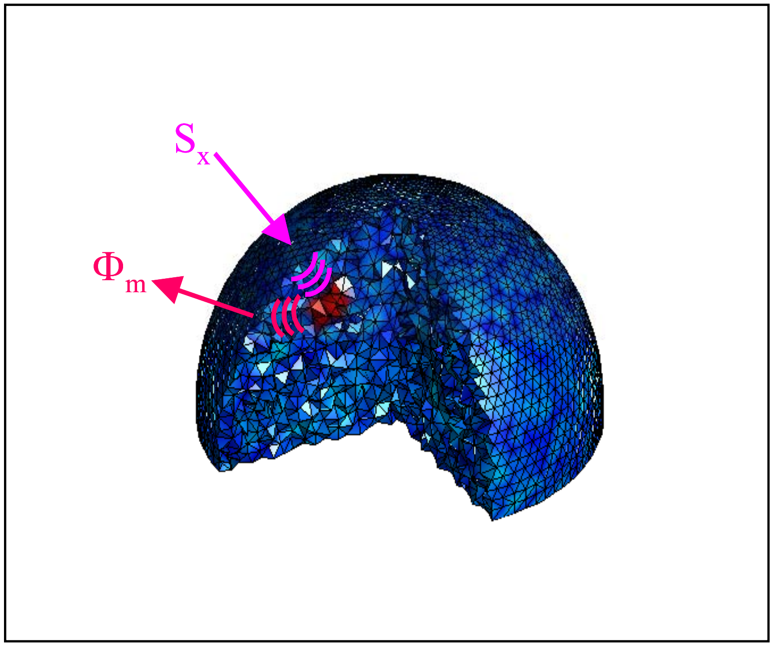


University of Vermont, Burlington, VT 05405

FREQUENCY-DOMAIN PHOTON MIGRATION PDE's

$$-\nabla \bullet \left(D_x \nabla \Phi_x\right) + k_x \Phi_x = S_x$$

$$-\nabla \bullet \left(D_m \nabla \Phi_m\right) + k_m \Phi_m = \beta \Phi_x$$



$$\begin{cases} D_x \dfrac{\partial \Phi_x}{\partial n} + r_x \Phi_x = 0 \\ \\ D_m \dfrac{\partial \Phi_m}{\partial n} + r_m \Phi_m = 0 \end{cases} \quad on \quad \partial\Omega$$

GENERALIZED FOURIER EXPANSION IN SPHERICAL COORDINATES

$$-\nabla \bullet \left(D_x \nabla \Phi_x\right) + k_x \Phi_x = S_x$$

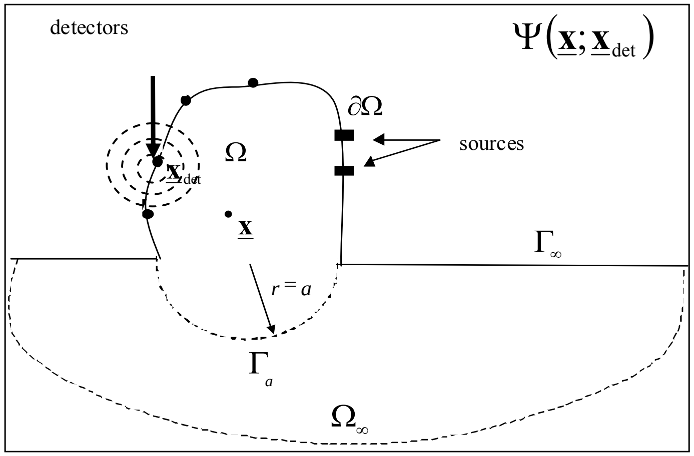
$$-\nabla \bullet \left(D_m \nabla \Phi_m\right) + k_m \Phi_m = \beta \Phi_x$$

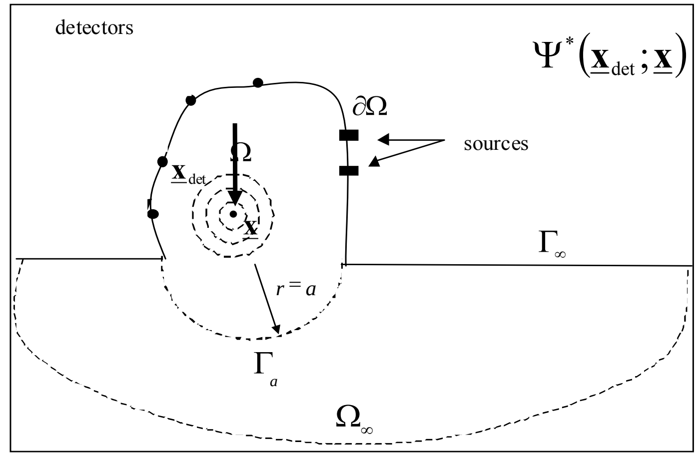
$$\Phi_x(r,\theta,\phi) = \sum A_{nm} \exp\left(im\theta\right) P_n^m(\phi) \frac{J_{n+1/2}(\sqrt{-k_x / D_x} r)}{\sqrt{r}}$$

$$\Phi_m(r,\theta,\phi) =$$

$$\sum \exp\left(im\theta\right) P_n^m(\phi) \left[B_{nm} \frac{J_{n+1/2}(\sqrt{-k_m / D_m} r)}{\sqrt{r}} - \frac{\beta / D_m}{k_x / D_x - k_m / D_m} A_{nm} \frac{J_{n+1/2}(\sqrt{-k_x / D_x} r)}{\sqrt{r}} \right]$$

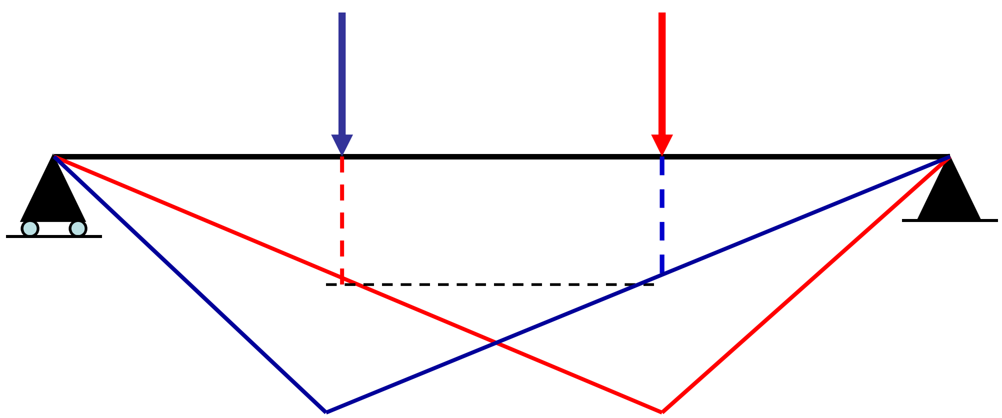
GREEN'S FUNCTION AND THE FUNDAMENTAL SOLUTION FOR SELF-ADJOINT OPERATORS



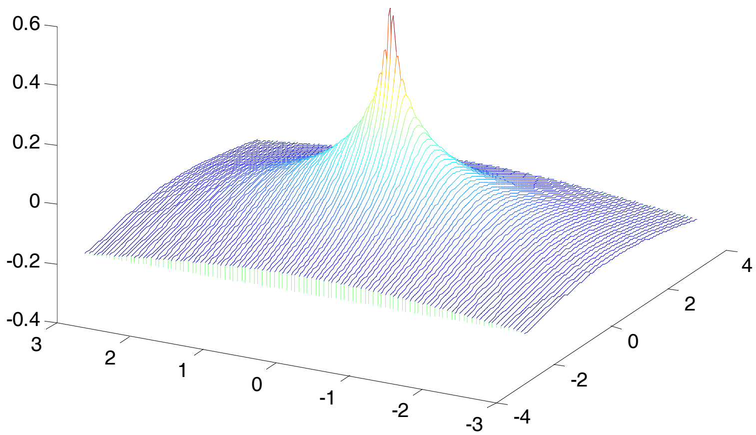


$$L(\Psi)=\delta(\underline{x}-\underline{x}_{det})$$

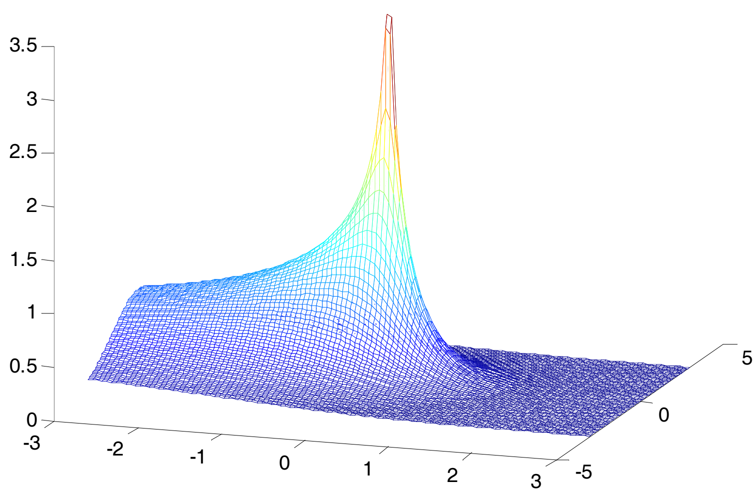
$$L^*(\Psi)=\delta(\underline{x}-\underline{x}_{det})$$



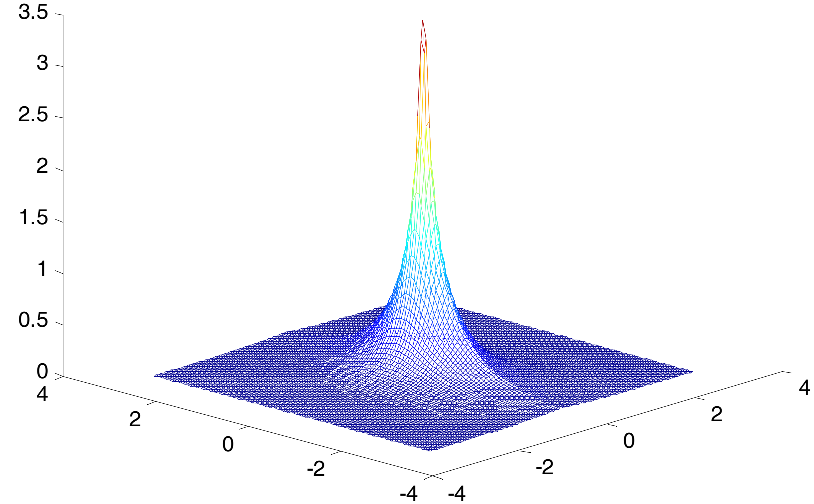
High diffusion



High convection



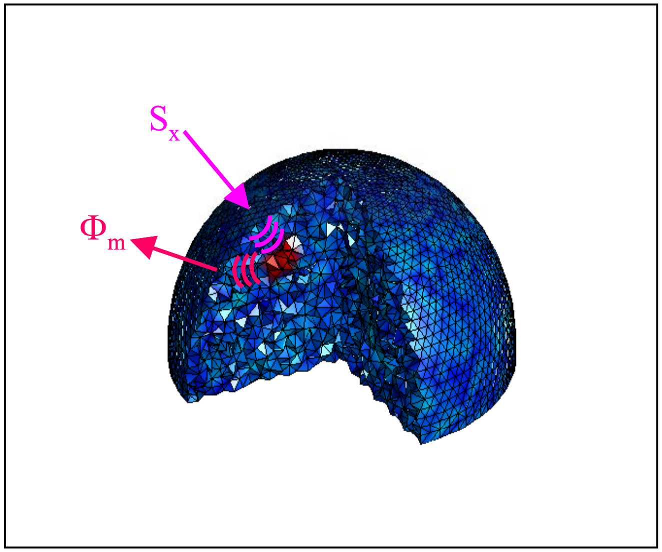
High reaction



GOVERNING EQUATIONS

matrix formulation of coupled complex equations

$$\begin{cases} -\underline{\underline{\nabla}}^t\left(\underline{\underline{\mathbf{d}}}\,\underline{\underline{\nabla}}\,\underline{\mathbf{\Phi}}\right)+\underline{\underline{\mathbf{k}}}\,\underline{\mathbf{\Phi}}=\underline{\mathbf{S}} \quad \textbf{on} \quad \Omega \\ \underline{\underline{\mathbf{D}}}\dfrac{\partial\underline{\mathbf{\Phi}}}{\partial n}+\underline{\underline{\mathbf{r}}}\,\underline{\mathbf{\Phi}}=\underline{0} \quad \textbf{on} \quad \partial\Omega \end{cases}$$



$$\underline{\underline{\nabla}}\equiv\begin{bmatrix}\nabla & \underline{0}\\ \underline{0} & \nabla\end{bmatrix};\quad \underline{\underline{\mathbf{d}}}\equiv\begin{bmatrix}D_x\underline{\underline{\mathbf{I}}} & \underline{\underline{\mathbf{0}}}\\ \underline{\underline{\mathbf{0}}} & D_m\underline{\underline{\mathbf{I}}}\end{bmatrix};\underline{\underline{\mathbf{D}}}\equiv\begin{bmatrix}D_x & 0\\ 0 & D_m\end{bmatrix};\quad \underline{\underline{\mathbf{k}}}\equiv\begin{bmatrix}k_x & 0\\ -\beta & k_m\end{bmatrix};\quad \underline{\underline{\mathbf{r}}}\equiv\begin{bmatrix}r_x & 0\\ 0 & r_m\end{bmatrix};$$

$$\underline{\mathbf{\Phi}}\equiv\begin{bmatrix}\Phi_x\\ \Phi_m\end{bmatrix};\quad \underline{\mathbf{S}}\equiv\begin{bmatrix}S_x\\ 0\end{bmatrix}.$$

BOUNDARY ELEMENT METHOD FOR DIFFUSION-REACTION SYSTEMS

Multiply by an arbitrary matrix $\underline{\underline{\Psi}}^t$

$$\int_\Omega \underline{\underline{\boldsymbol{\Psi}}}^t\left(-\underline{\underline{\nabla}}^t\left(\underline{\underline{\nabla}}\,\underline{\boldsymbol{\Phi}}\right)+\underline{\underline{\mathbf{d}}}^{-1}\underline{\underline{\mathbf{k}}}\,\underline{\boldsymbol{\Phi}}\right)d\Omega=\int_\Omega \underline{\underline{\boldsymbol{\Psi}}}^t\,\underline{\underline{\mathbf{d}}}^{-1}\underline{\mathbf{S}}\,d\Omega$$

Integration by parts twice

$$\int_\Omega\left(-\underline{\underline{\nabla}}^t\left(\underline{\underline{\nabla}}\,\underline{\underline{\boldsymbol{\Psi}}}\right)+\left(\underline{\underline{\mathbf{d}}}^{-1}\underline{\underline{\mathbf{k}}}\right)^t\underline{\underline{\boldsymbol{\Psi}}}\right)^t\underline{\boldsymbol{\Phi}}\,d\Omega+\int_{\partial\Omega}\left(-\underline{\underline{\boldsymbol{\Psi}}}^t\frac{\partial\underline{\boldsymbol{\Phi}}}{\partial \boldsymbol{n}}+\frac{\partial\underline{\underline{\boldsymbol{\Psi}}}}{\partial \boldsymbol{n}}\underline{\boldsymbol{\Phi}}\right)d\boldsymbol{S}=\int_\Omega\underline{\underline{\boldsymbol{\Psi}}}^t\,\underline{\underline{\mathbf{d}}}^{-1}\underline{\boldsymbol{S}}\,d\Omega$$

Term involving volume integral of the unknown $\underline{\boldsymbol{\Phi}}$

"Green matrix"

$$-\underline{\underline{\nabla}}^t\left(\underline{\underline{\nabla}}\,\underline{\underline{\boldsymbol{\Psi}}}\right)+\left(\underline{\underline{\mathbf{d}}}^{-1}\underline{\underline{\mathbf{k}}}\right)^t\underline{\underline{\boldsymbol{\Psi}}}+\underline{\underline{\boldsymbol{\delta}}}=0$$

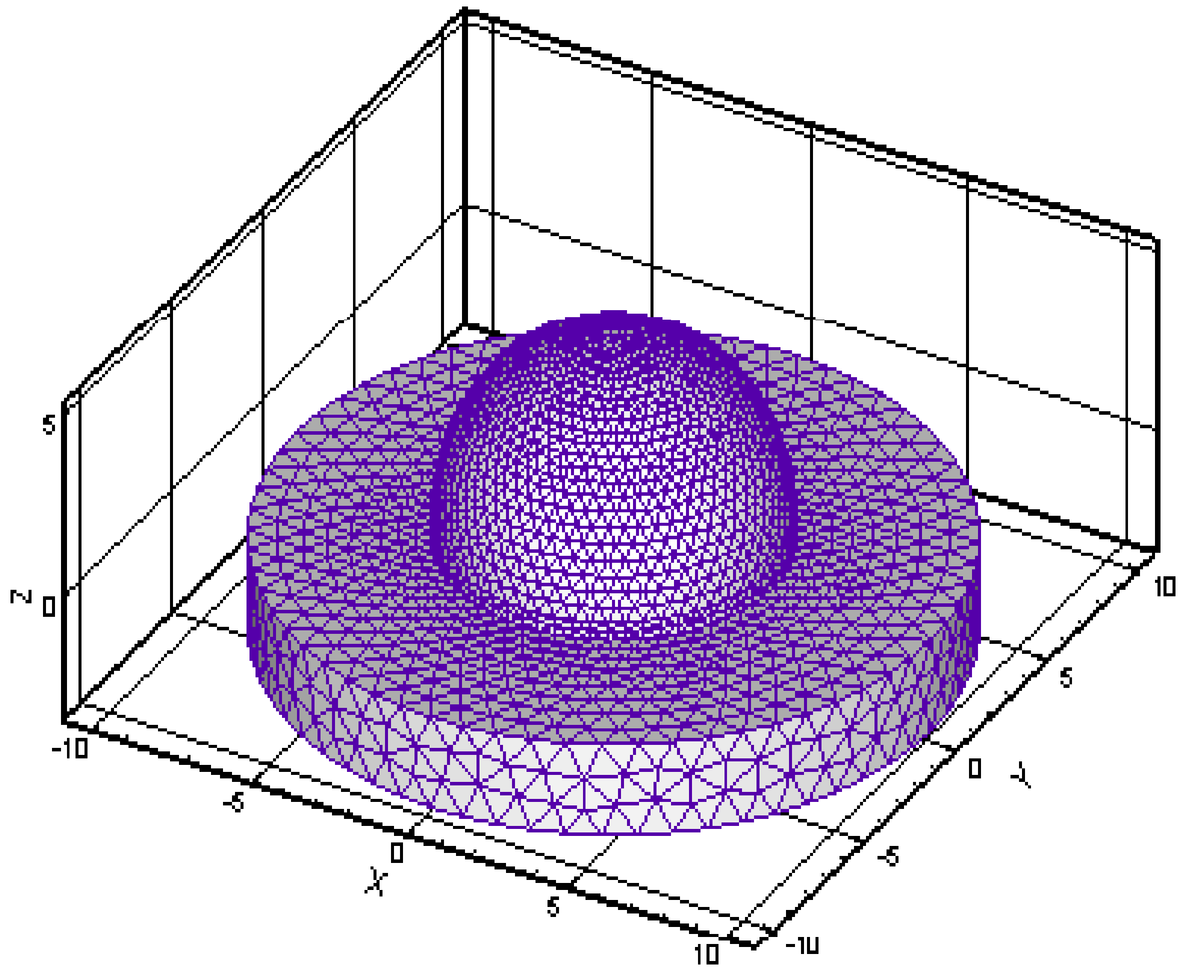
THE GREEN MATRIX

Choose $\underline{\underline{\Psi}}$ to be the ***"Green matrix"*** by putting a Dirac source $\underline{\mathbf{x}}_0$ at the boundary points

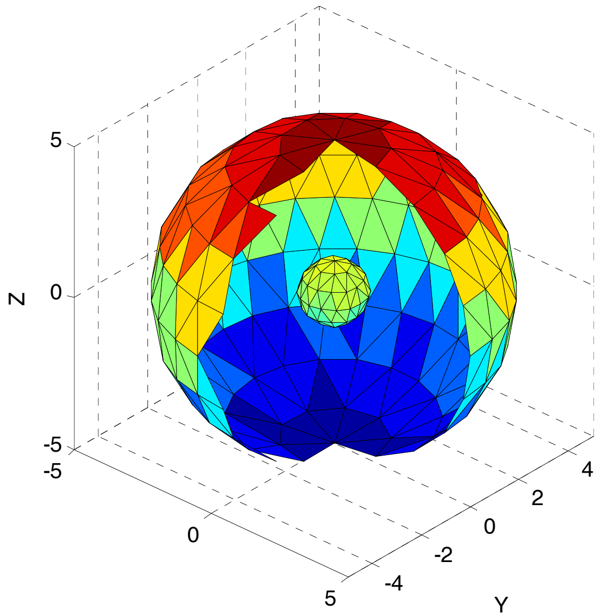
$$\frac{1}{2}\underline{\mathbf{\Phi}}(\underline{x}_0)+\int_{\partial\Omega}\left(-\underline{\underline{\mathbf{\Psi}}}^t\frac{\partial\underline{\mathbf{\Phi}}}{\partial n}+\frac{\partial\underline{\underline{\mathbf{\Psi}}}}{\partial n}\underline{\mathbf{\Phi}}\right)dS=\int_{\Omega}\underline{\underline{\mathbf{\Psi}}}^t\,\underline{\underline{\mathbf{d}}}^{-1}\underline{S}\,d\Omega$$

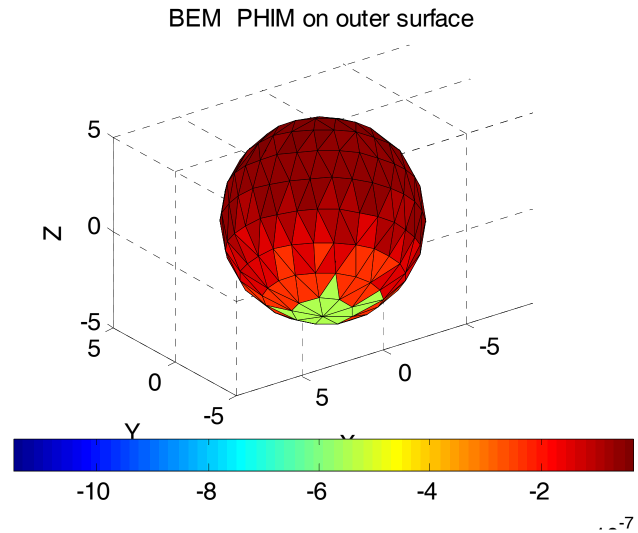
$$\underline{\underline{\mathbf{\Psi}}}(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}}_0)=\begin{bmatrix}\dfrac{\exp(-\boldsymbol{i}\lambda_1|\underline{\boldsymbol{x}}-\underline{\boldsymbol{x}}_0|)}{4\pi|\underline{\boldsymbol{x}}-\underline{\boldsymbol{x}}_0|} & 0\\ \alpha\left(\dfrac{\exp(-\boldsymbol{i}\lambda_2|\underline{\boldsymbol{x}}-\underline{\boldsymbol{x}}_0|)}{4\pi|\underline{\boldsymbol{x}}-\underline{\boldsymbol{x}}_0|}-\dfrac{\exp(-\boldsymbol{i}\lambda_1|\underline{\boldsymbol{x}}-\underline{\boldsymbol{x}}_0|)}{4\pi|\underline{\boldsymbol{x}}-\underline{\boldsymbol{x}}_0|}\right) & \dfrac{\exp(-\boldsymbol{i}\lambda_2|\underline{\boldsymbol{x}}-\underline{\boldsymbol{x}}_0|)}{4\pi|\underline{\boldsymbol{x}}-\underline{\boldsymbol{x}}_0|}\end{bmatrix}$$

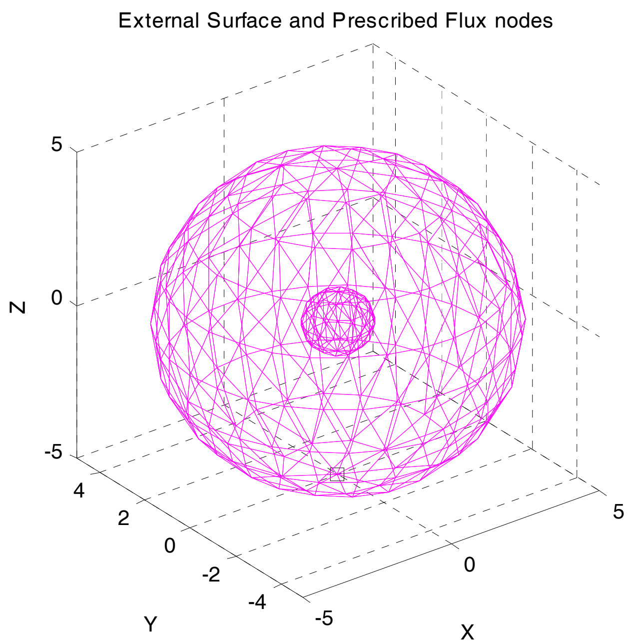
BOUNDARY ELEMENT MESH

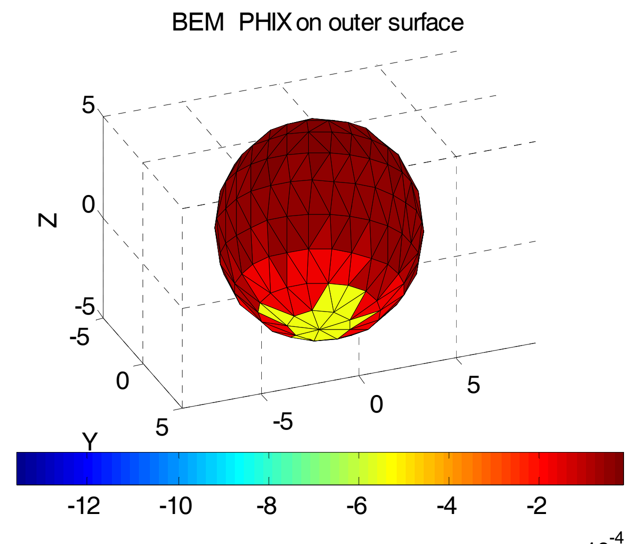


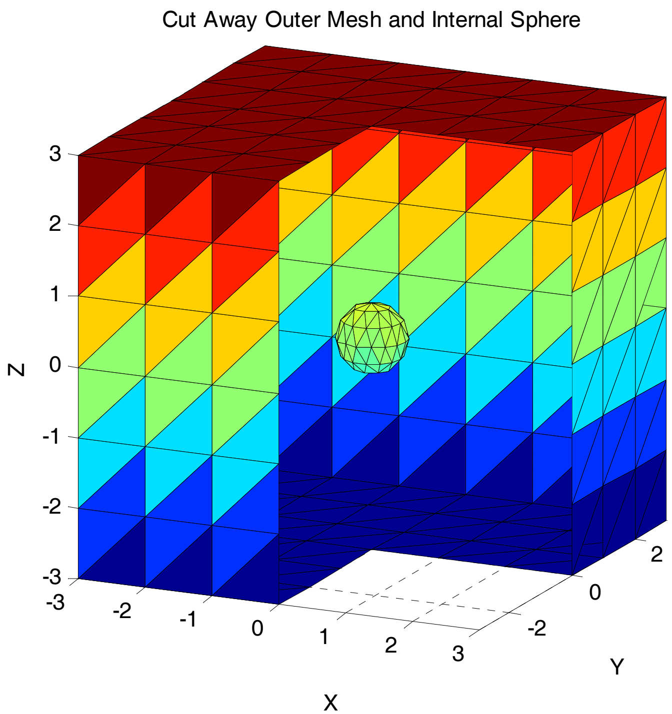
SOME APPLICATIONS

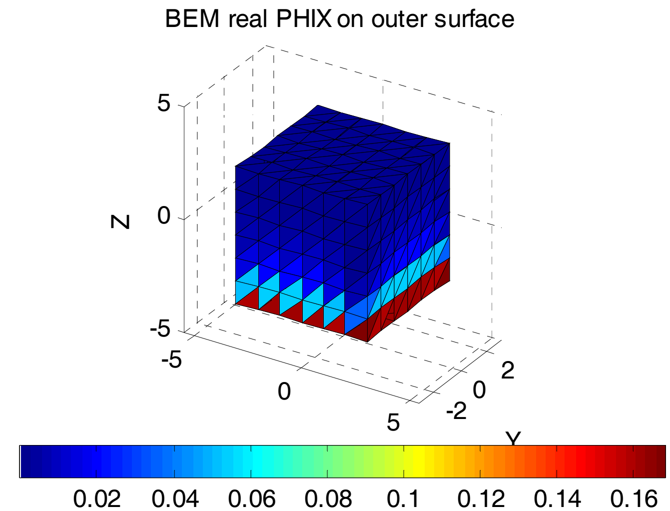


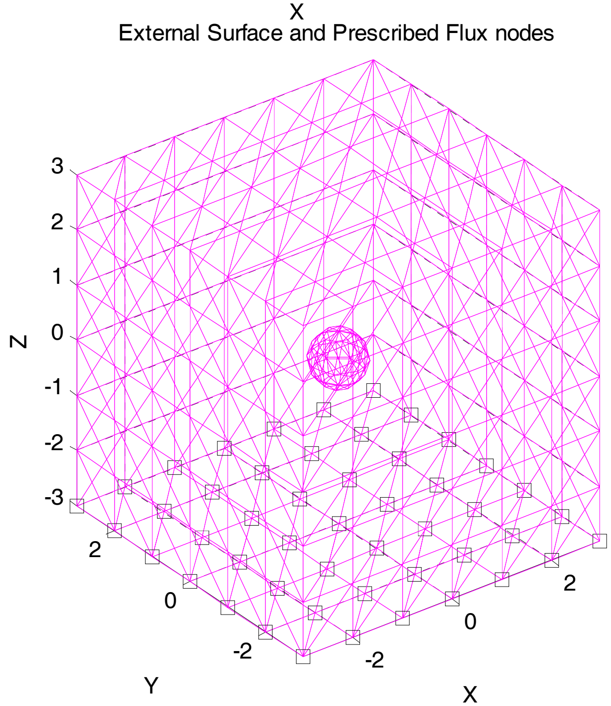


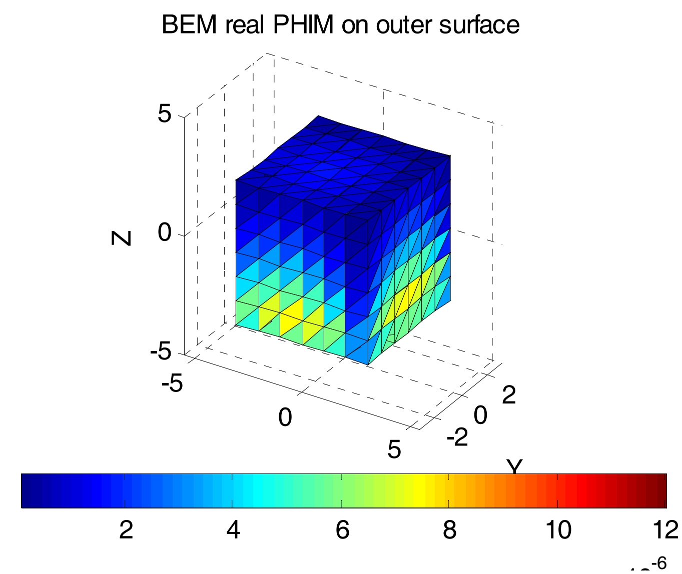





Cut Away Outer Mesh and Internal Sphere
Z
X
Y


BEM real PHIX on outer surface
Z
Y
0.02 0.04 0.06 0.08 0.1 0.12 0.14 0.16


External Surface and Prescribed Flux nodes
Z
Y
X


BEM real PHIM on outer surface
Z
Y
2 4 6 8 10 12

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Gail
Hania, Laurel, Vannette

My family