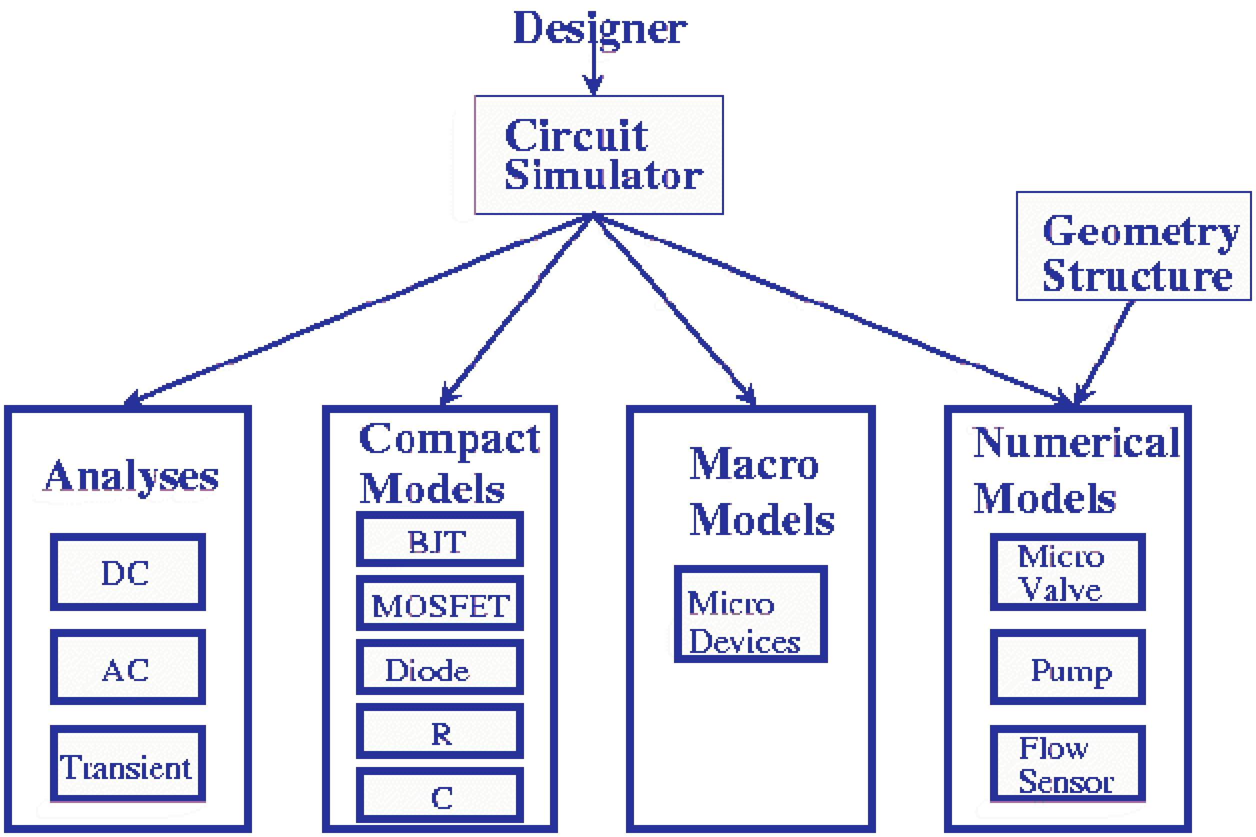
Topics

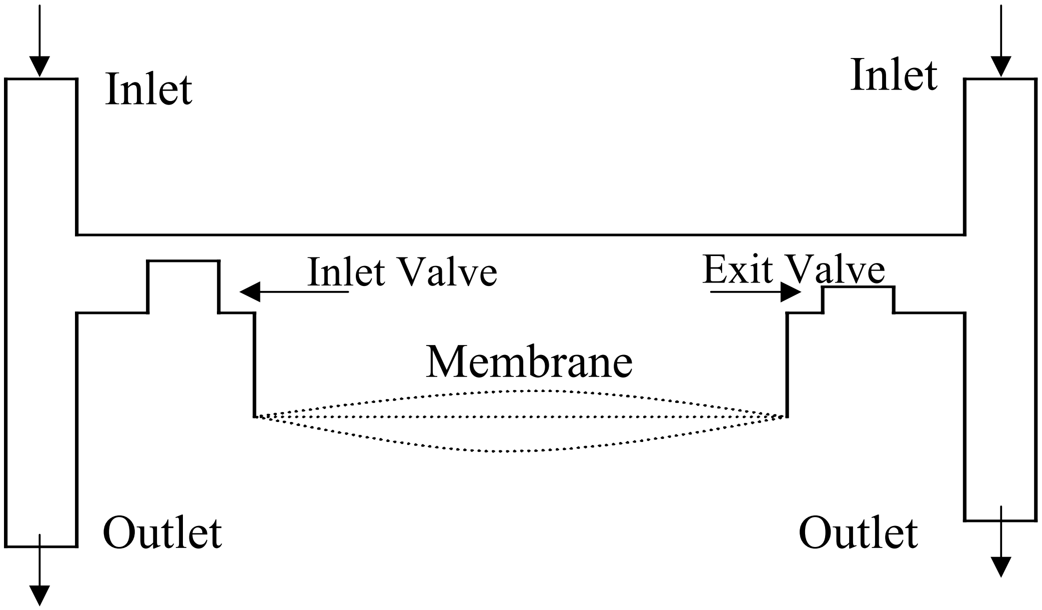
- Full-systems MEMS modeling
- Flow Solver-NEKTAR
- Chaotic Advection
- Stochastic Modeling

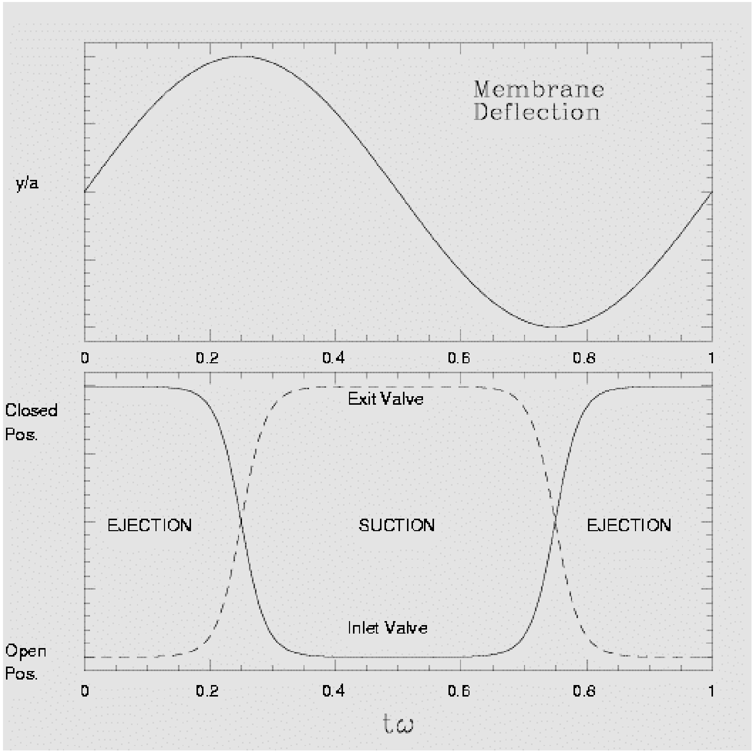
(Mikuchenko & Mayaram, 2000)

Coupled Circuit/Device Simulator

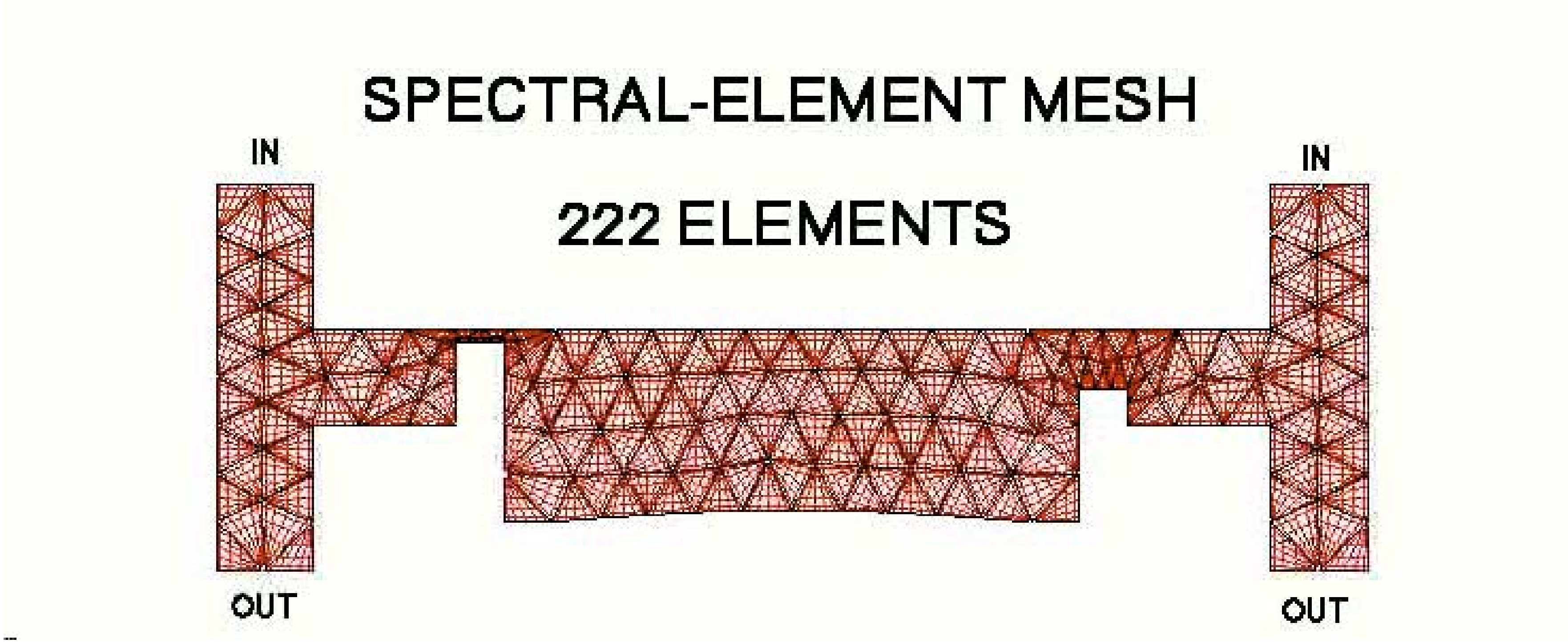


Micro Device Concepts and Simulation Based Verification: Micro-Pump

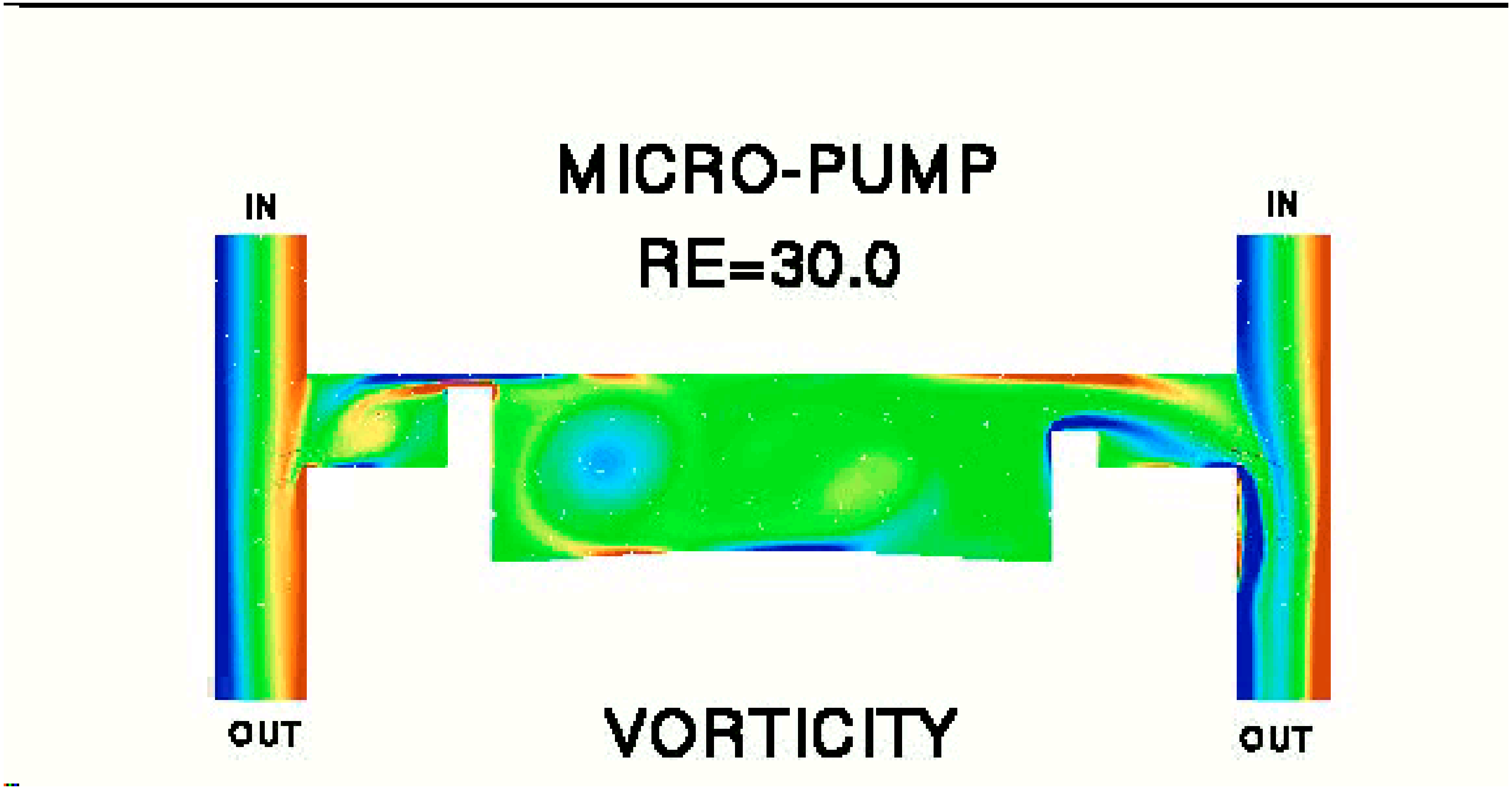




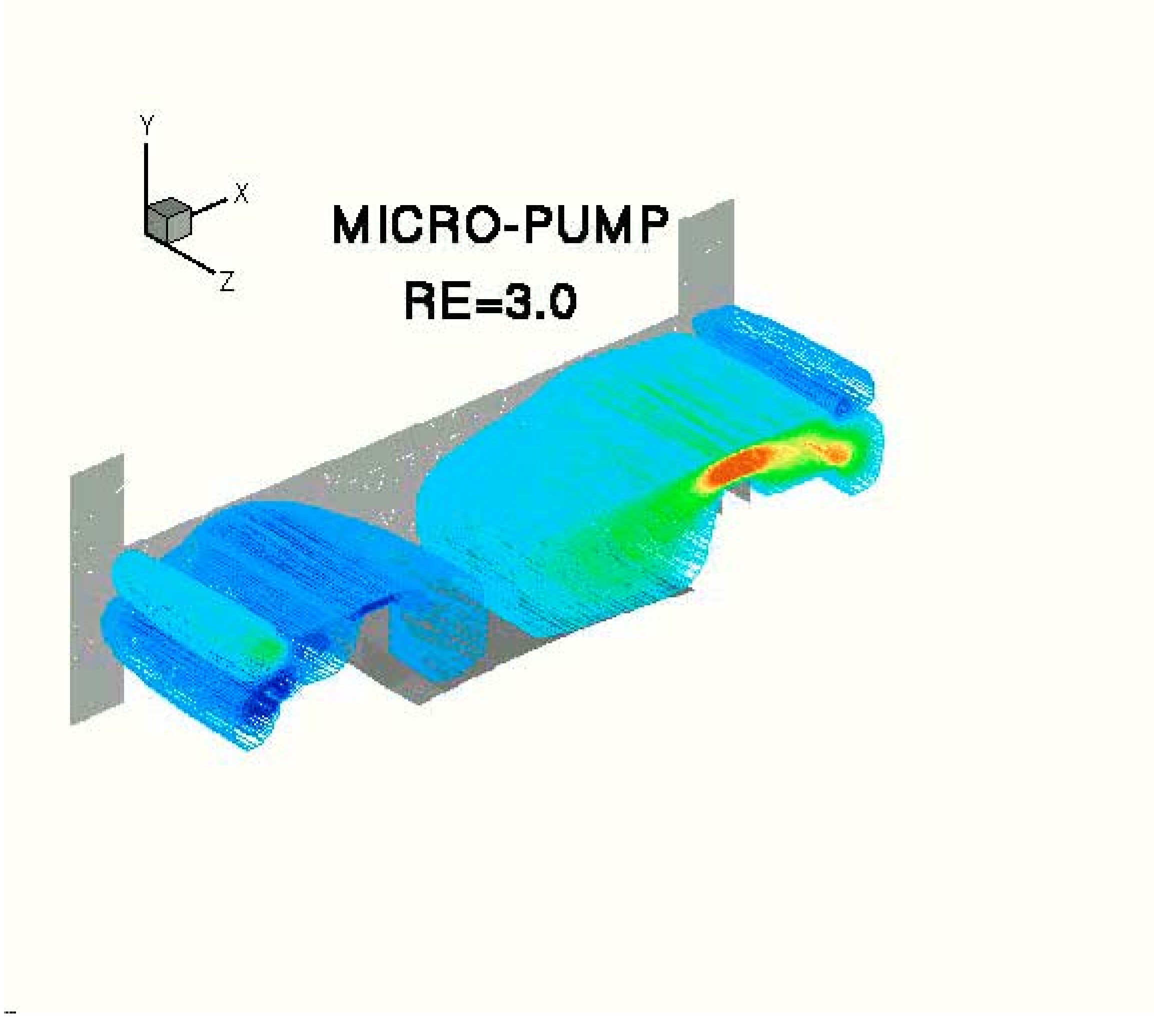
H/P Finite Element Method with Arbitrary Lagrangian Eulerian Formulation



Conceptual Design and Simulation of a Micro-Pump

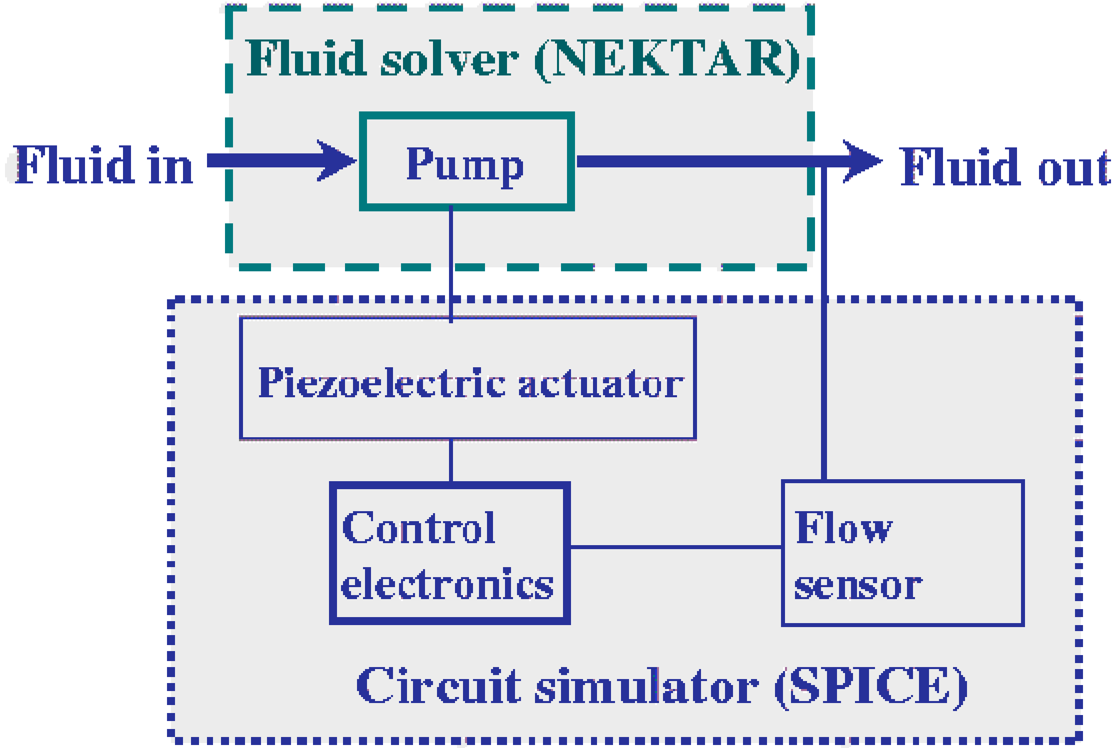


Conceptual Design and Simulation of a Micro-Pump (3-D Simulation)

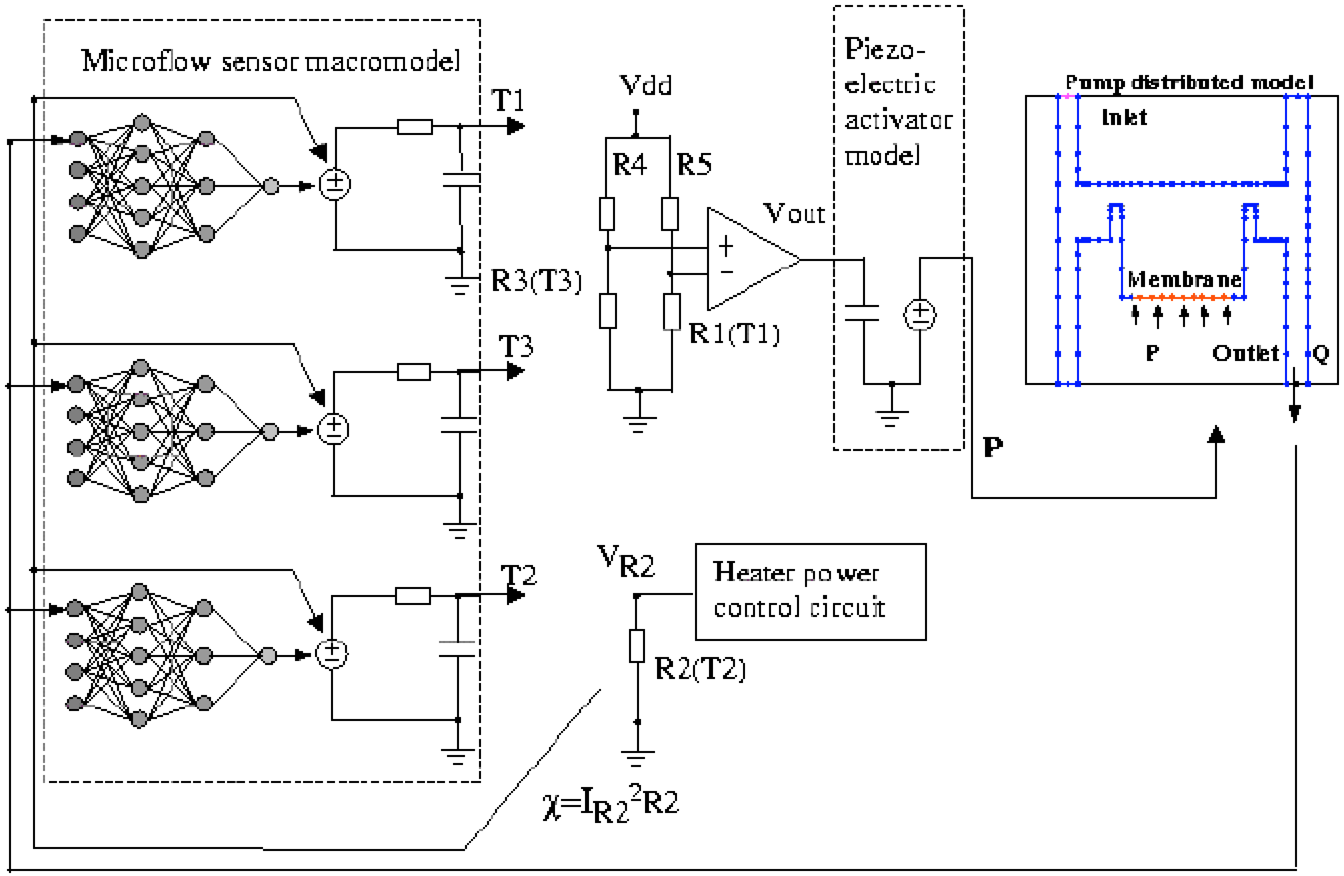


SPICE-NEKTAR Coupling

Direct Coupling: Simulator Interaction



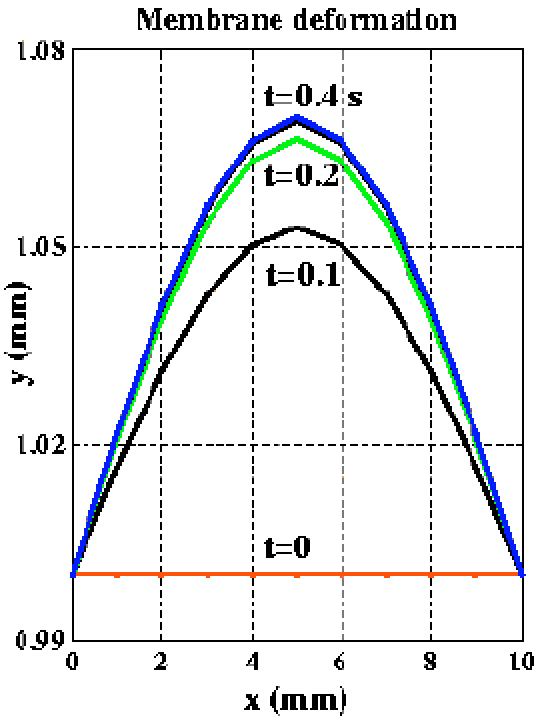
Microfluidic System Model

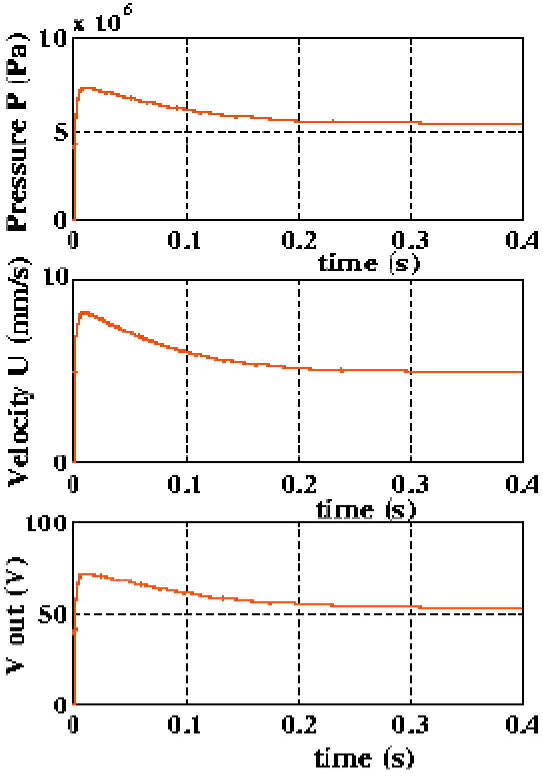


Time Stepping Scheme

- Fluid solver is called from SPICE
- The time step for SPICE < time step for fluid solver
- Fluid solver specifies the next synchronization time point
- Results: the number of fluid solver calls is the same as that of standalone fluid solver

Simulation Results





Simulation Results

Statistics SPICE / Nektar

Total iterations

7234 / 800

Transient timepoints

3567 / 800

Accepted timepoints

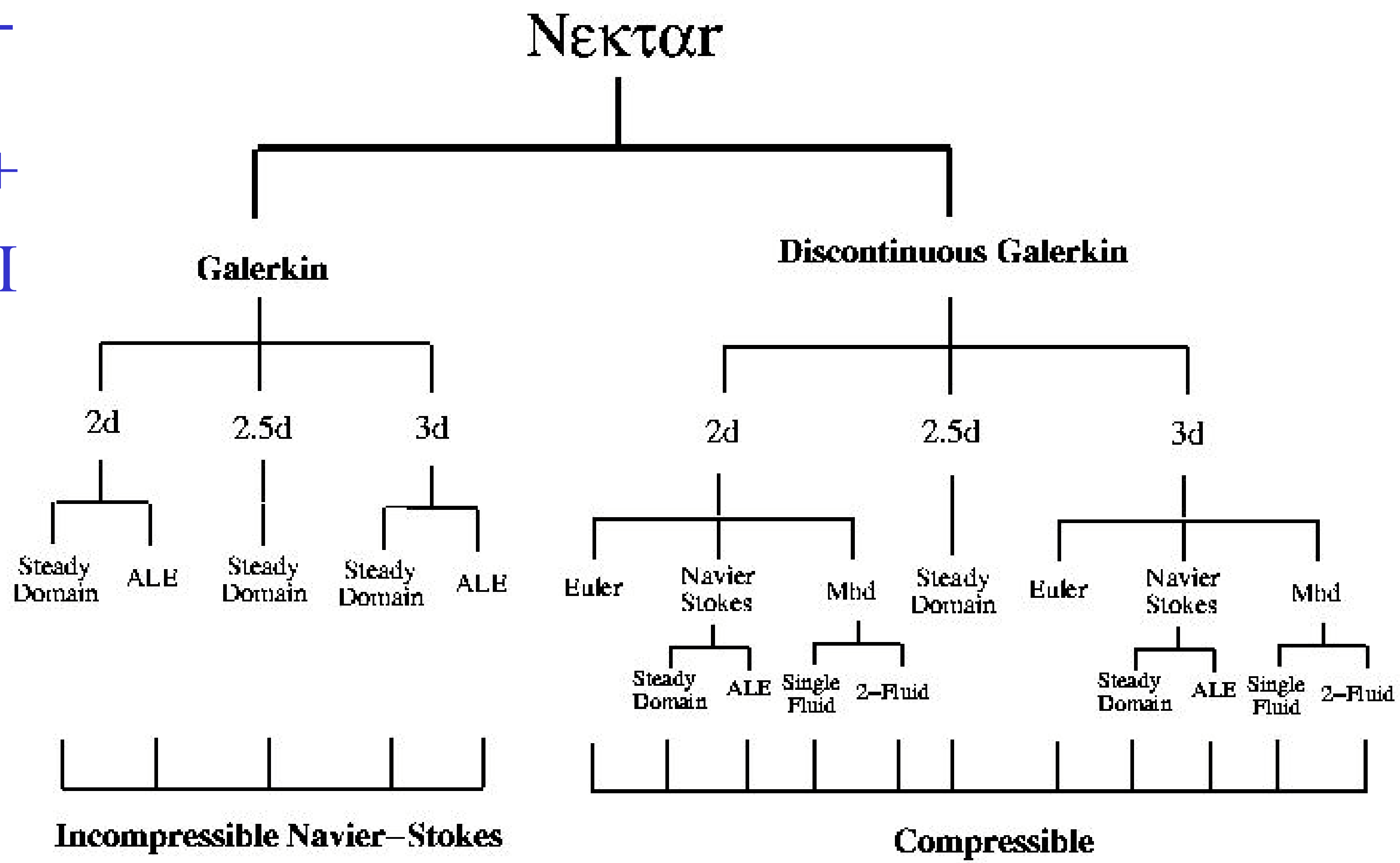
3562 / 800

Total Analysis Time

0.43s / 5min (PII - 300MHz)

Nεκταr Capabilities

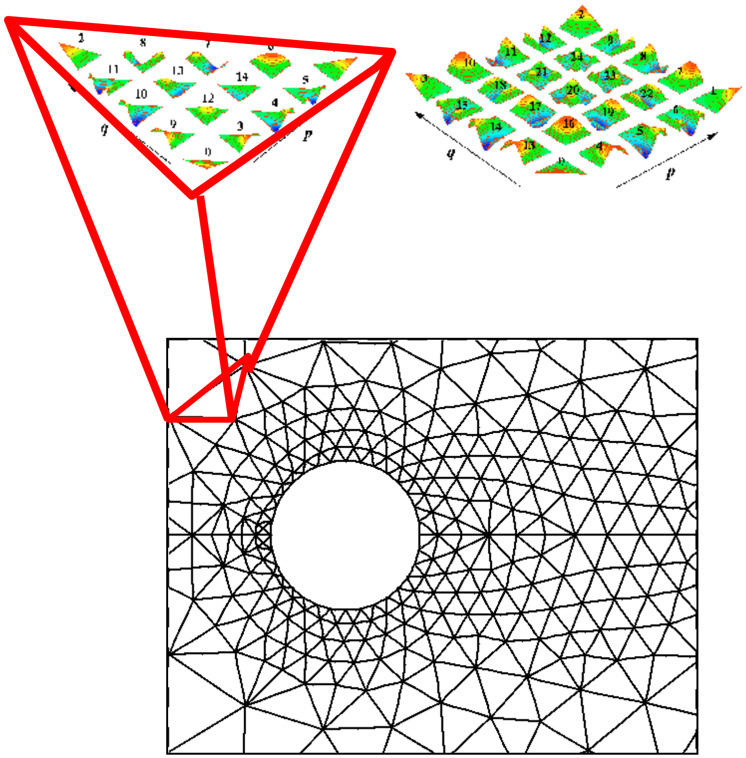
- **Open-Source**
- C++
- MPI



* The only high-order code for complex geometries

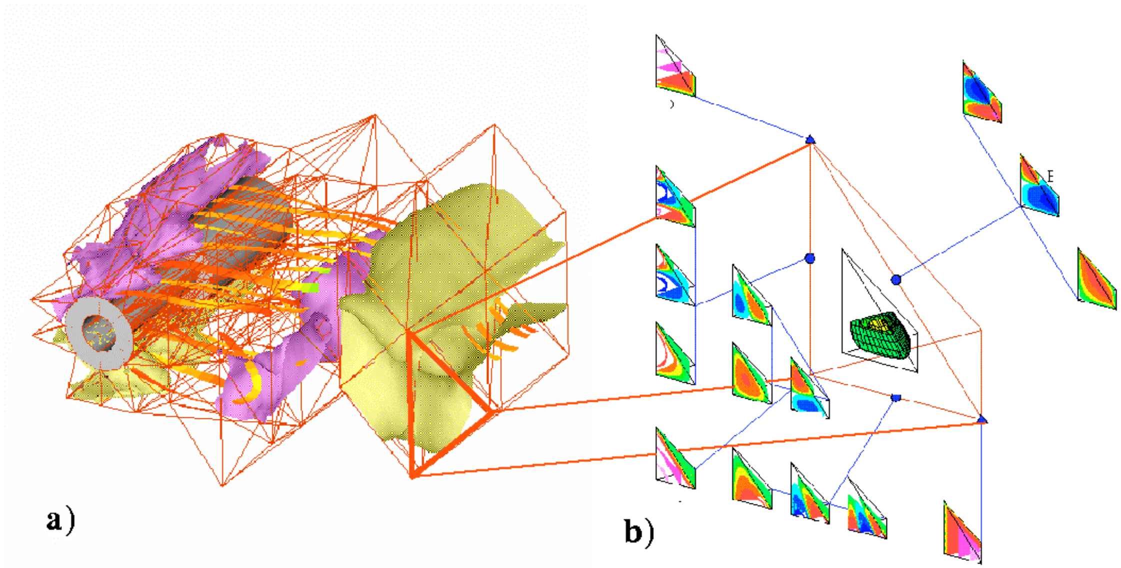
Spectral/*hp* Elements

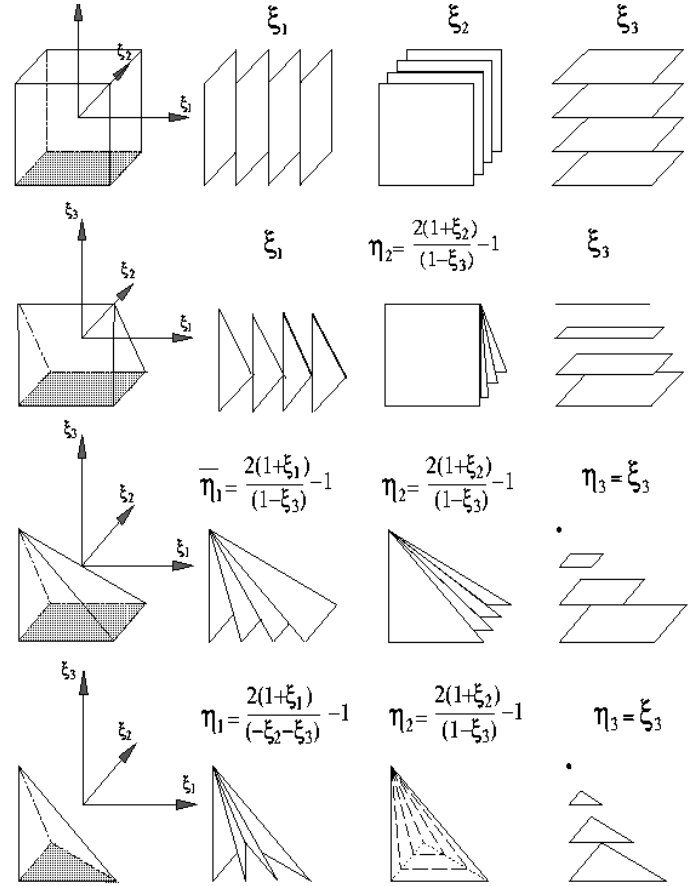
- Efficient discretization complex geometries
- Standard finite element meshes used
- Global spectral accuracy
- Resolution increased by increasing **P** or **element number**



Karniadakis & Sherwin, Spectral/hp Element Methods for CFD, Oxford University Press, 1999.

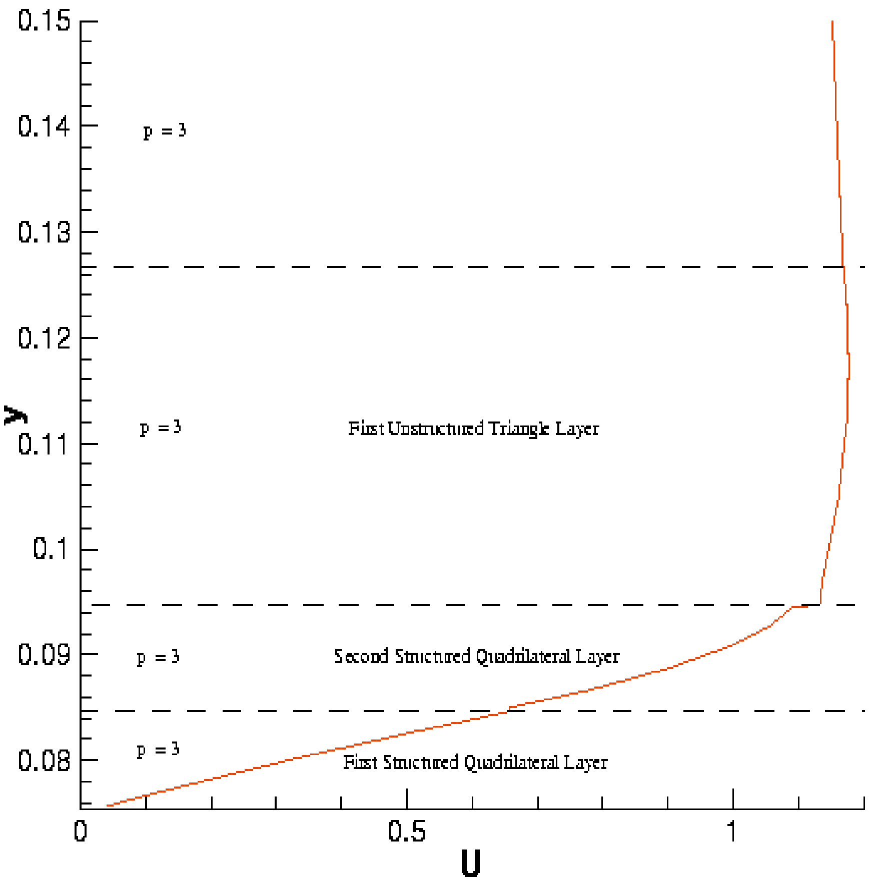
Method/Expansion Bases

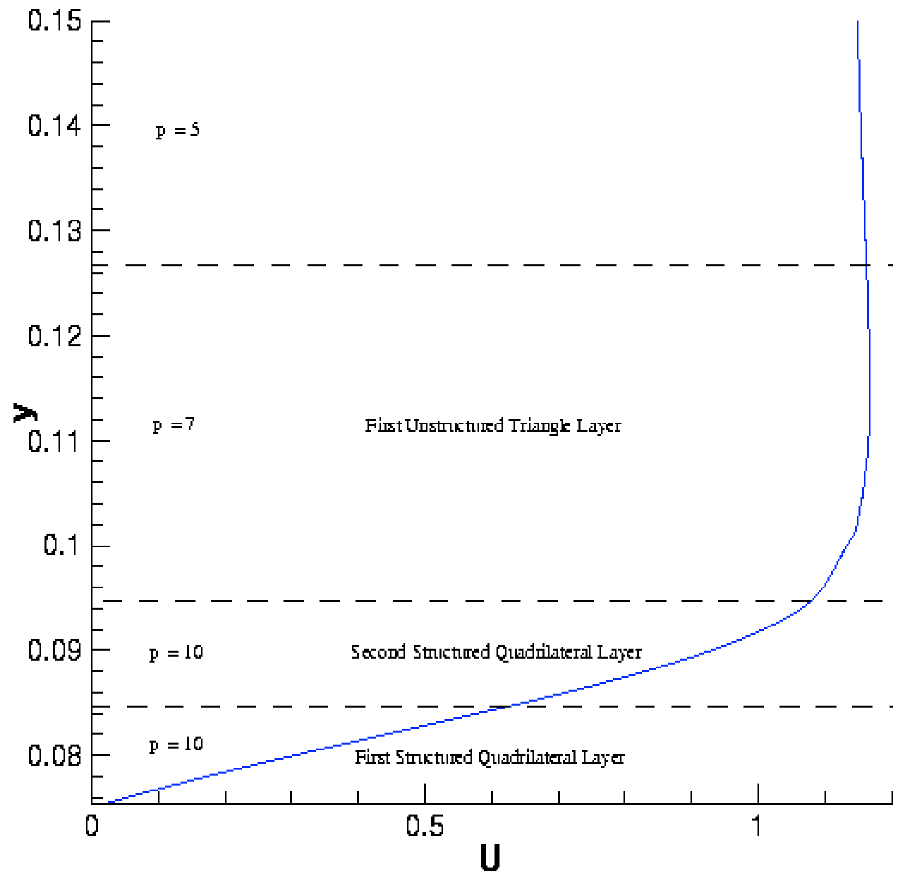




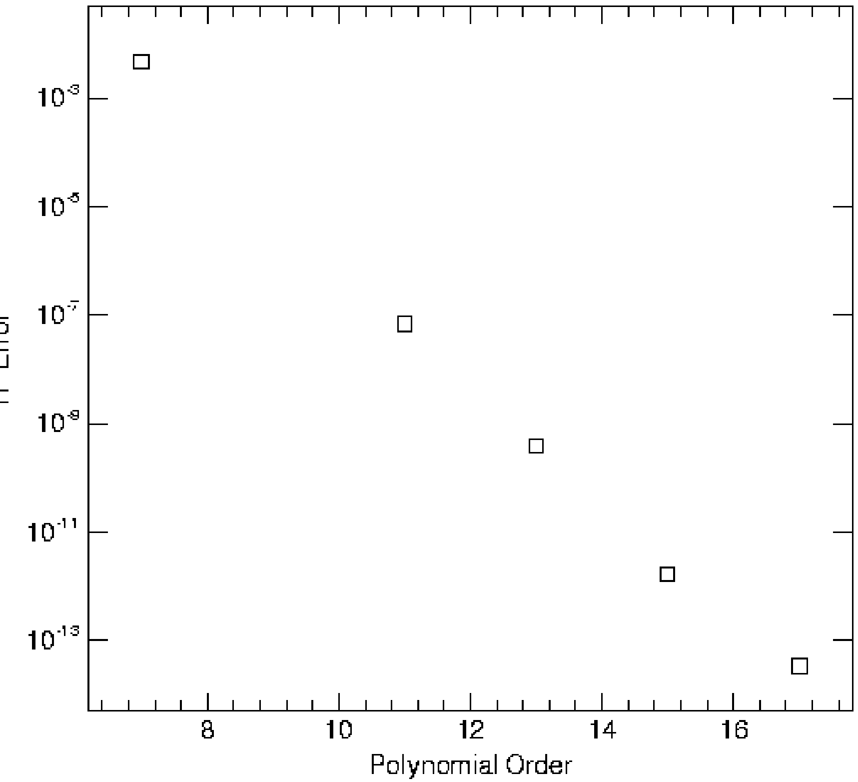
Spectral/hp Element Methods for CFD
Karniadakis & Sherwin,
Oxford University Press, 1999

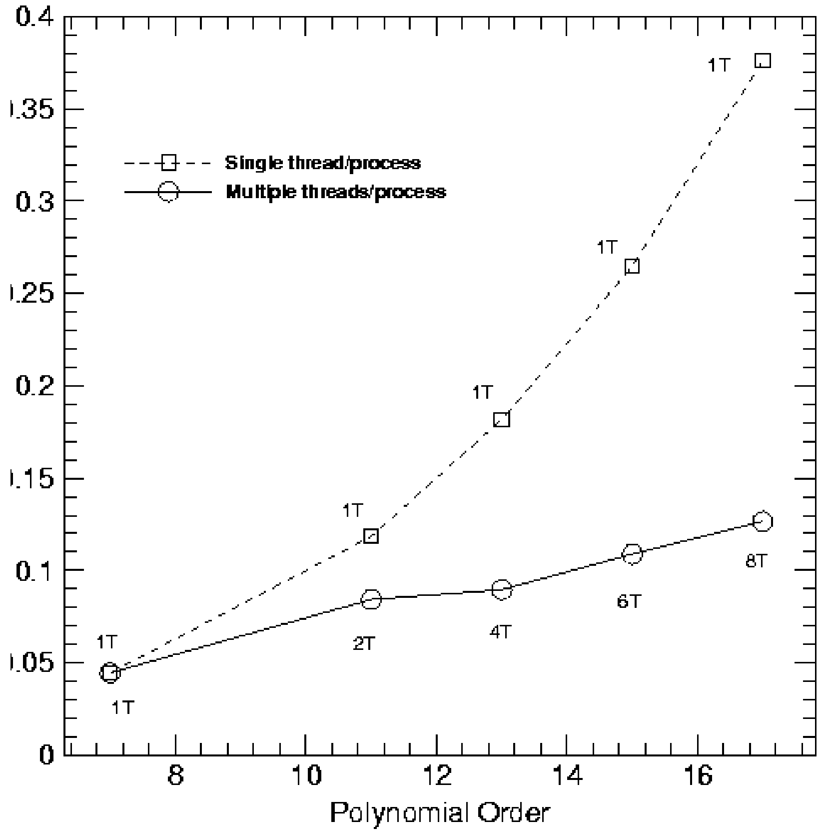
Variable Polynomial Order on Hybrid Elements





MPI/OpenMP NEKTAR





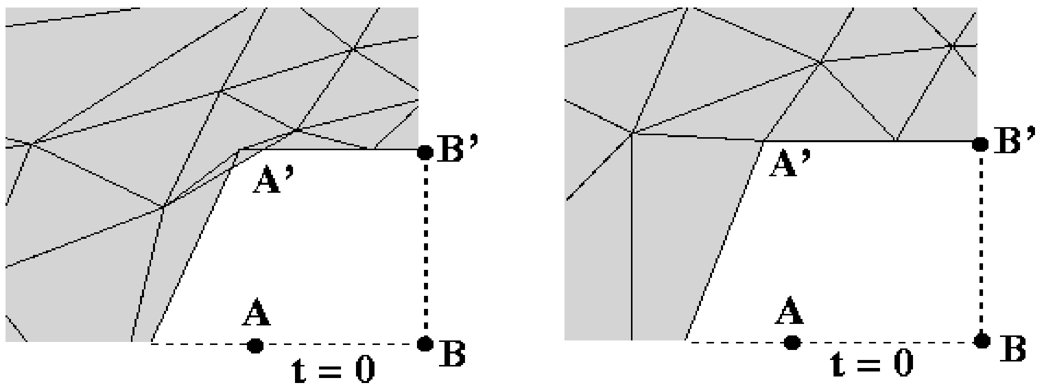
•Exponential accuracy at sublinear cost using Threads

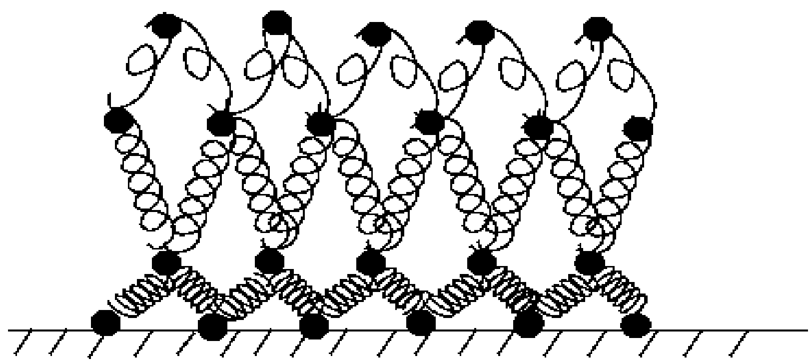
NEKTAR-ALE Formulation

- ALE = Arbitrary Lagrangian-Eulerian
- Introduces an “arbitrary” vertex velocity into the variational formulation
- Lagrangian at the structure boundary
- Eulerian on the domain boundary
- Seek a mesh velocity algorithm which
  - produces a smoothly varying mesh velocity
  - computationally efficient

Graph Theory Algorithm

The ALE Grid Velocity Algorithm

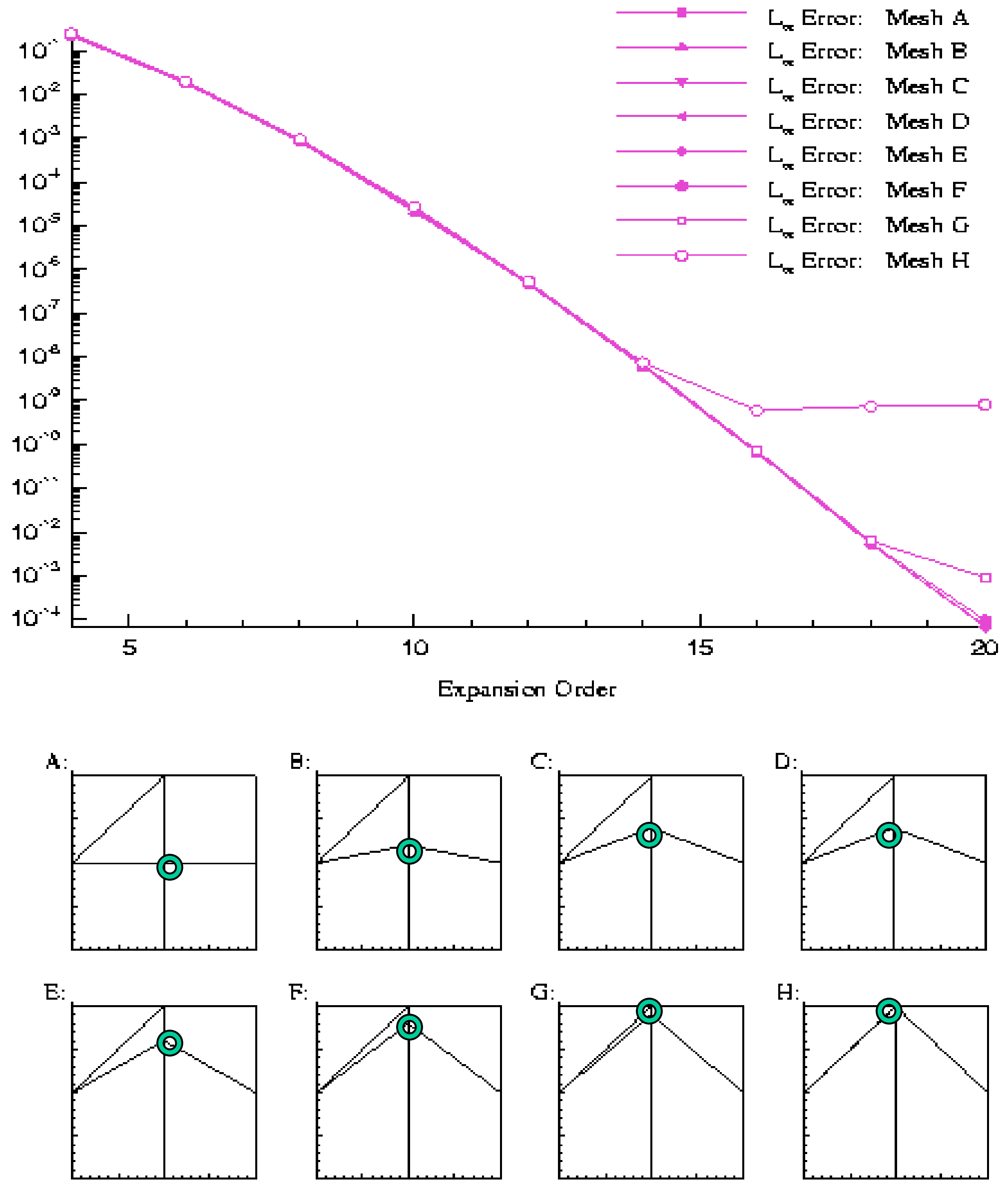




Graph Theory: Force Directed Method in Velocity Space

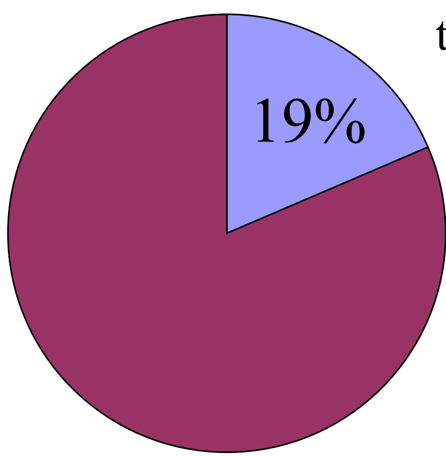
Fast Analog of $\nabla \bullet (\kappa \nabla Ug) = 0$ Using Incomplete Iteration

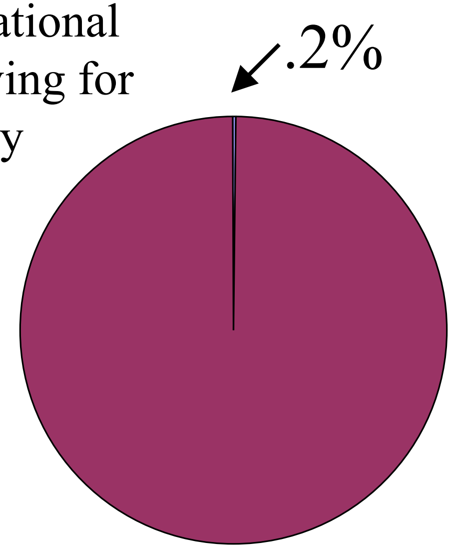
Convergence with Skewed Elements

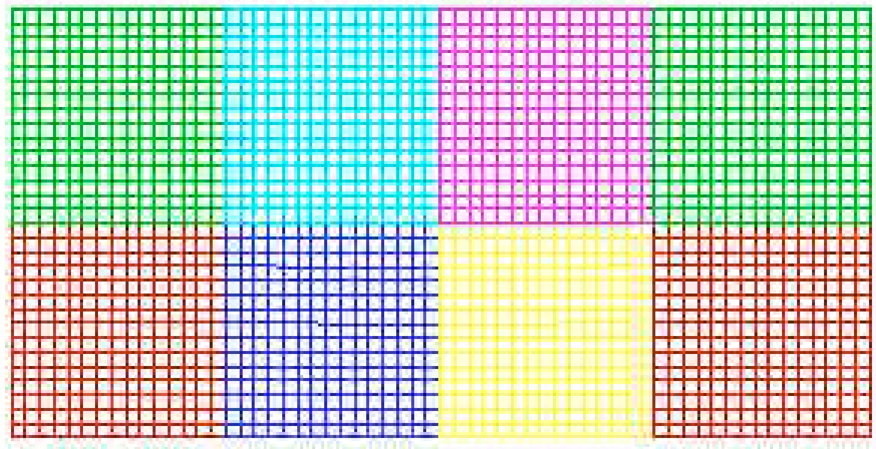


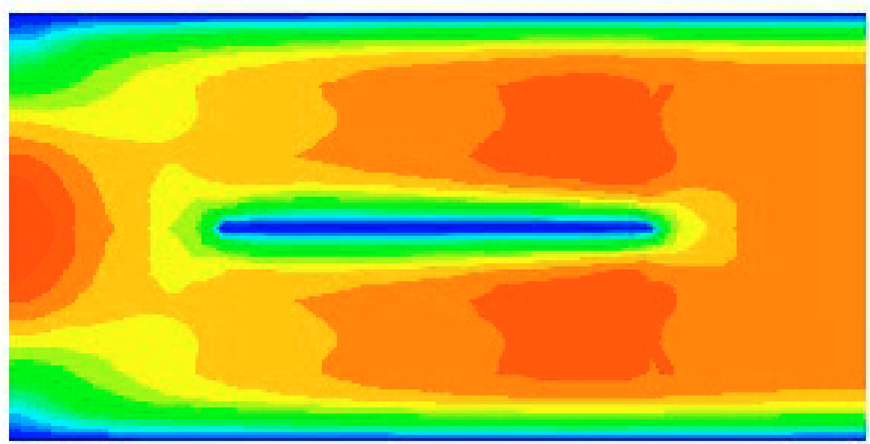
	Traditional Mesh Movement Algorithm		Graph Theory Based Algorithm	
Modal Order	Time Per Timestep	Time to Compute Mesh Velocity	Time Per Timestep	Time to Compute Mesh Velocity
4	3.416 s	.04753 s	3.044 s	0.02 s
6	7.882 s	1.4079 s	6.406 s	0.02 s
8	15.215 s	2.8495 s	12.291 s	0.02 s
10	32.451 s	10.53 s	22.956 s	0.02 s

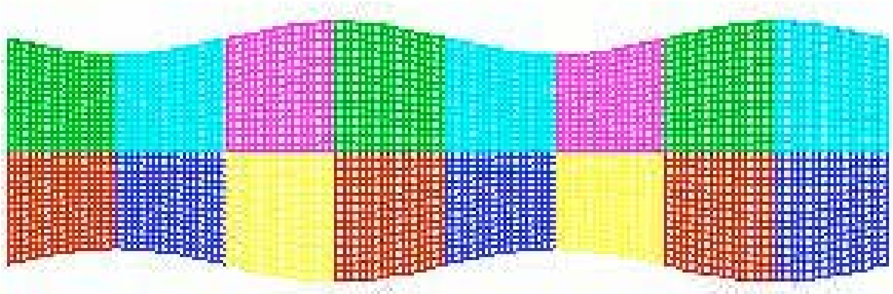
Percentage of Computational Time Dedicated to Solving for the Mesh Velocity

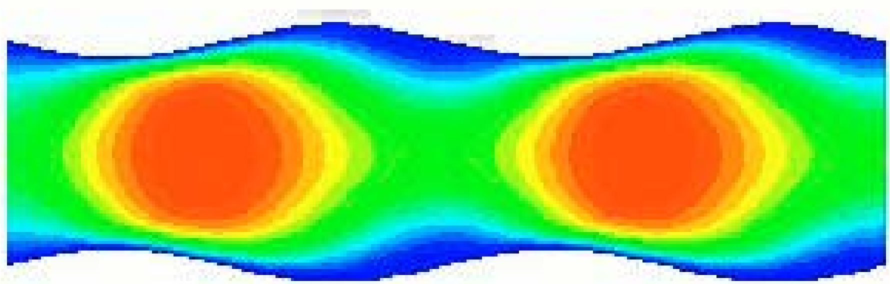






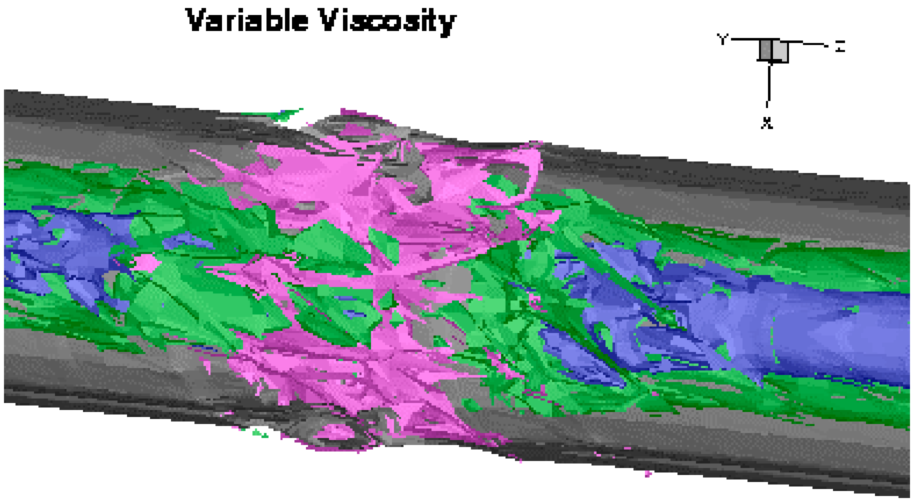


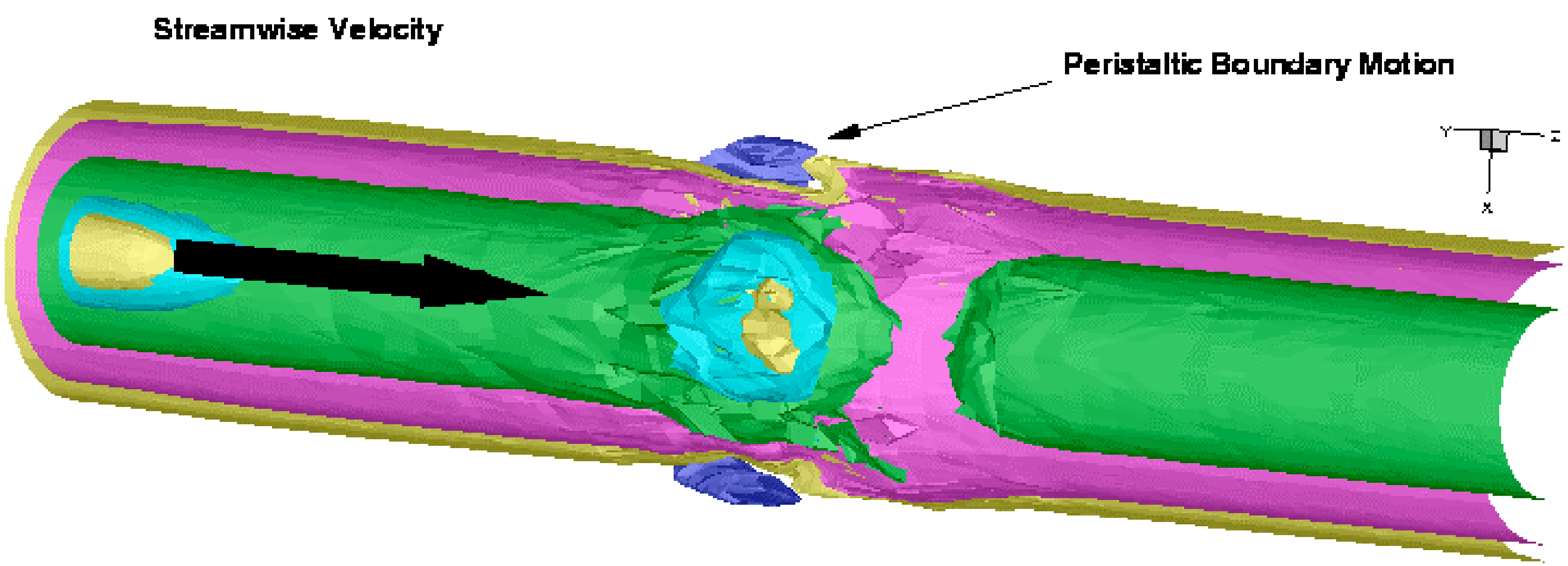




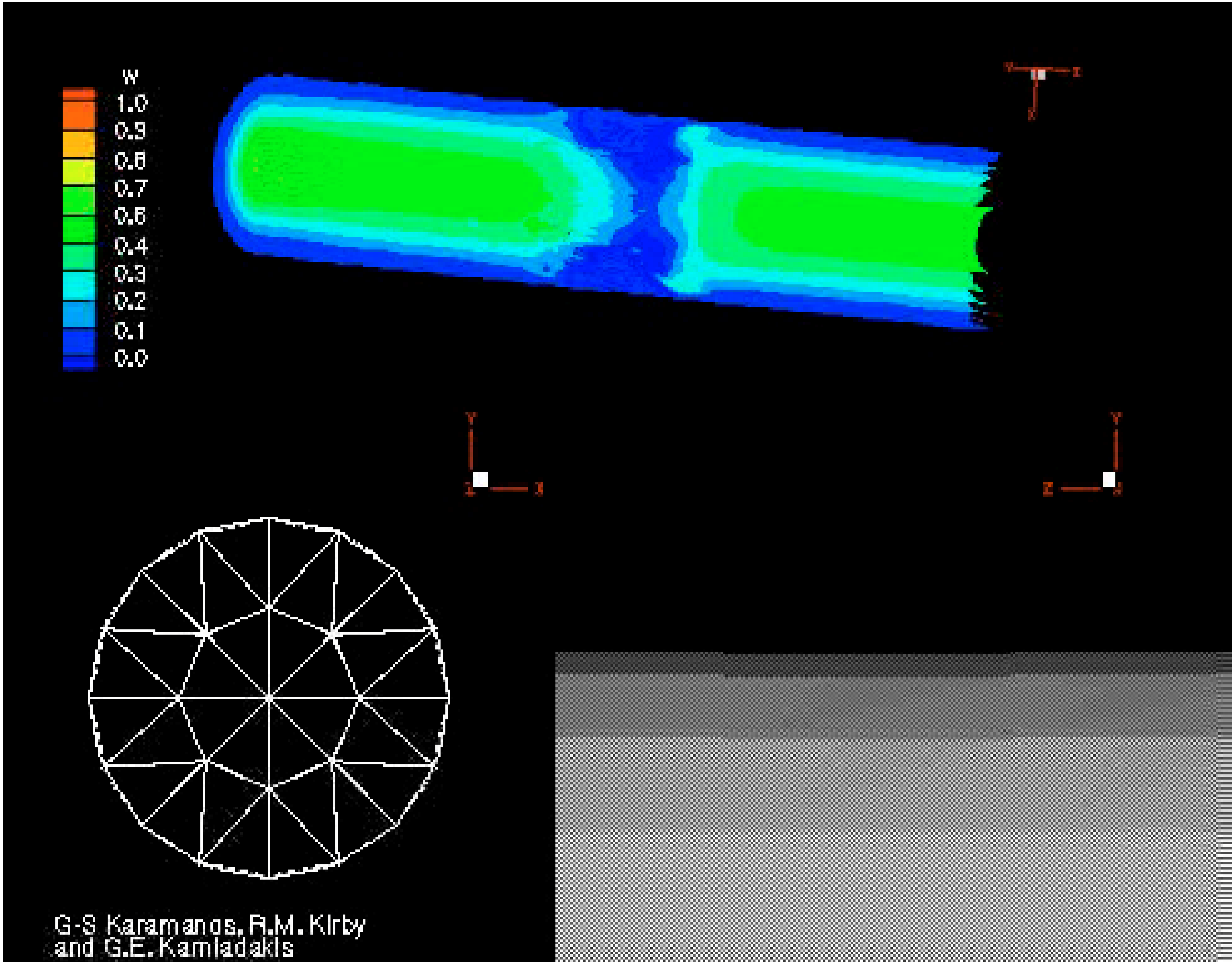
NEKTAR-ALE CODE

- **Non-Newtonian Micro-Fluids in Deforming Geometries**
- **Graph Theory Approach**

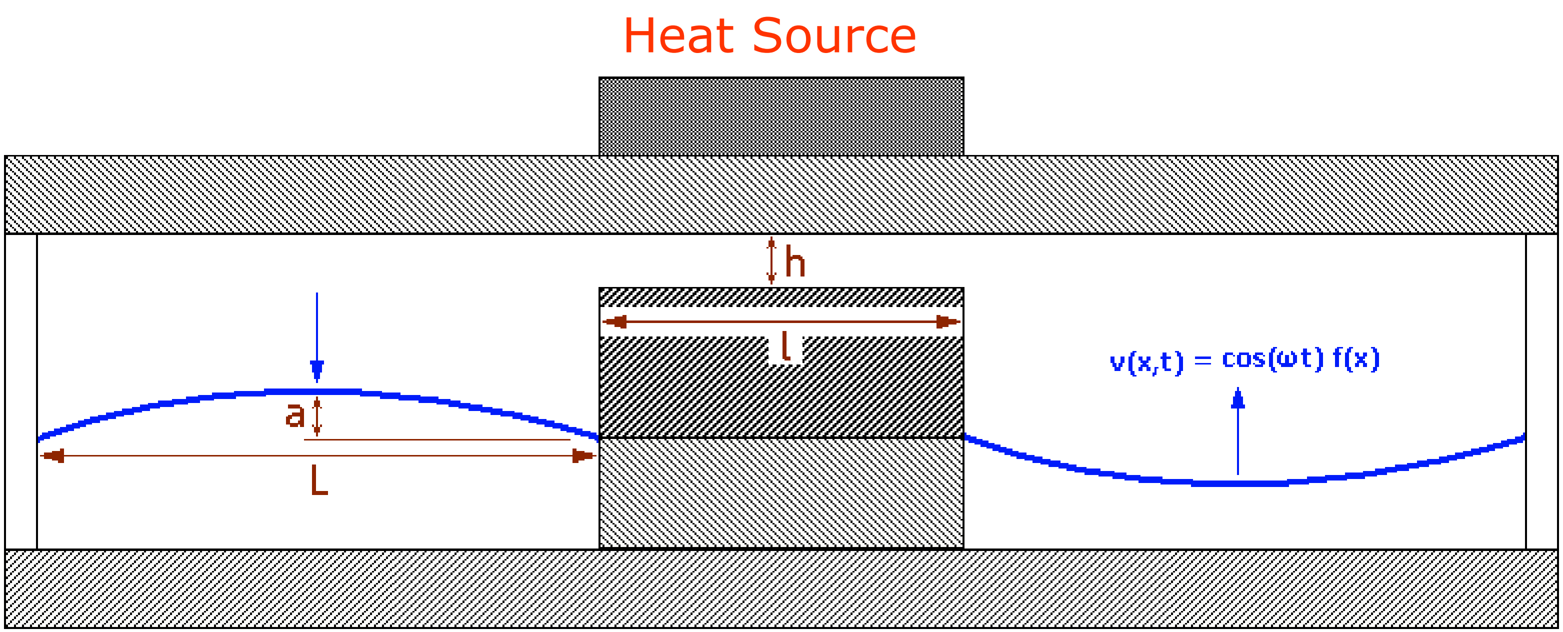




G-S Karamanos, R.M. Kirby and G.E. Karniadakis, Brown University

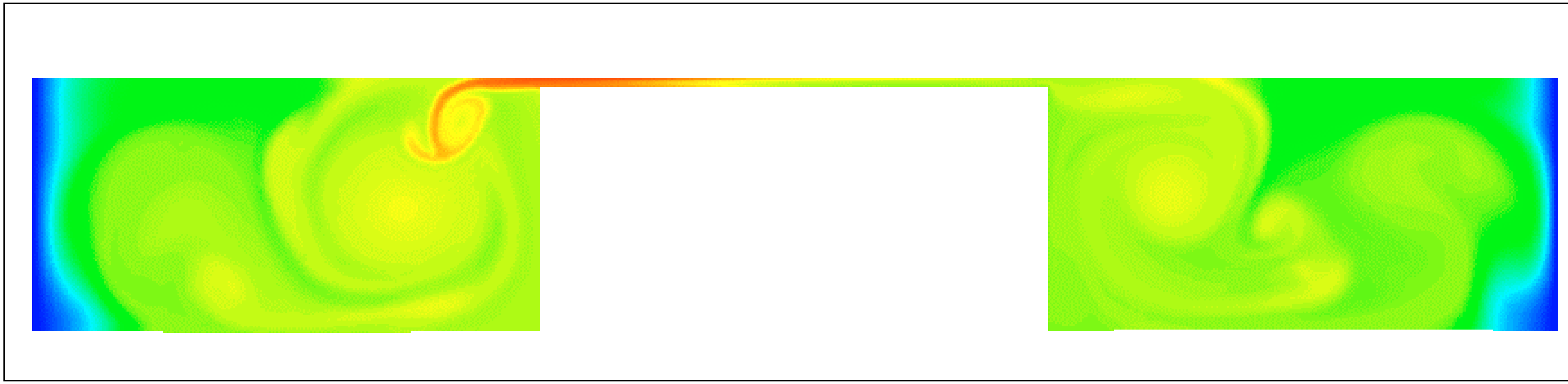

W
1.0
0.9
0.8
0.7
0.6
0.4
0.3
0.2
0.1
0.0
G-S Karamanos, R.M. Kirby
and G.E. Karniadakis

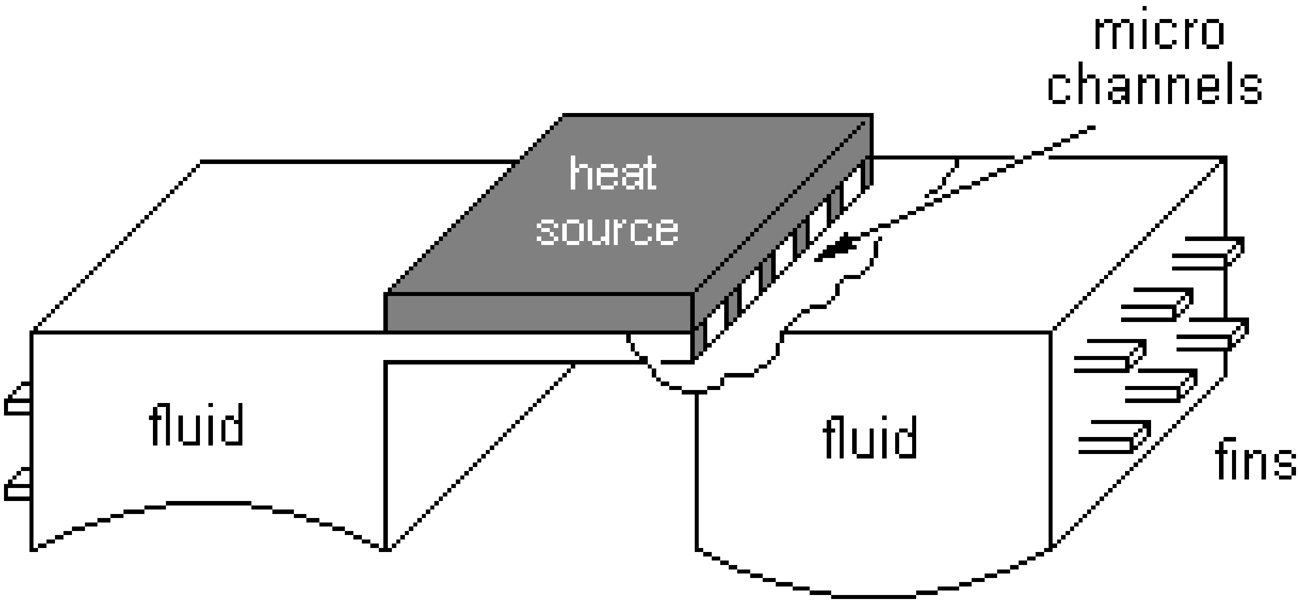
Micro Device Concepts and Simulation Based Verification: The Micro Heat Spreader



h : channel height
l : channel length
a : membrane oscillation amplitude
L : membrane length
ω : membrane oscillation frequency

CFD Based Design & Validation: Micro Heat Spreader

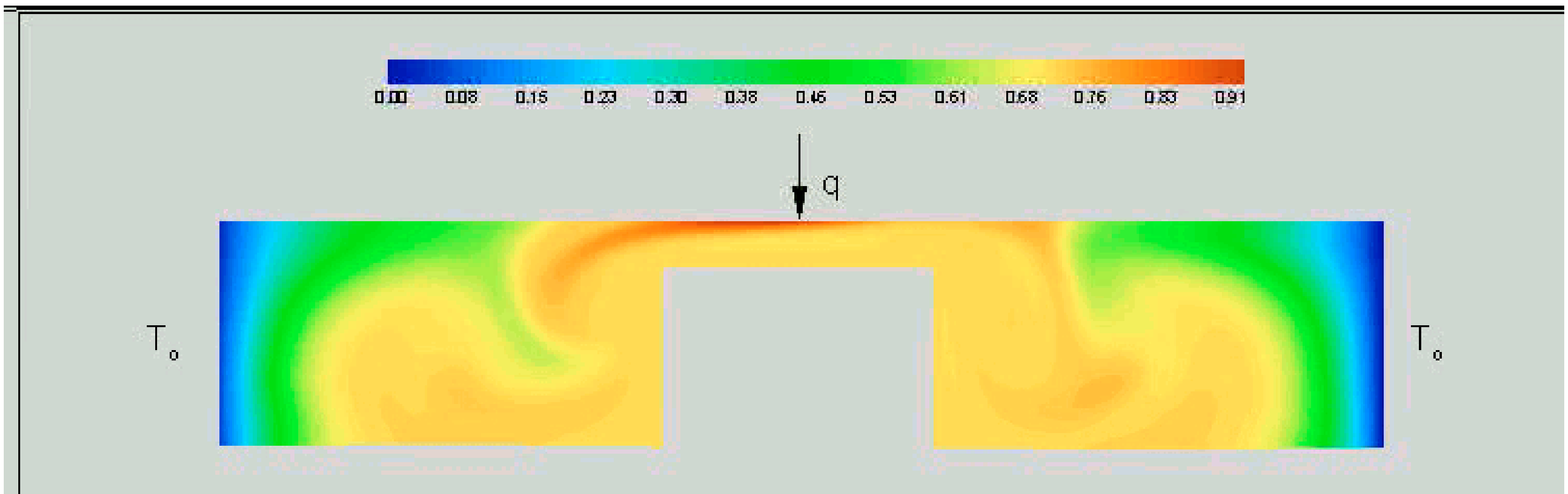




Micro Heat Spreaders: Reciprocating Flow Forced Convection

Micro Heat Spreaders, a Concept Verification

- **Very high heat flux removal** $\left(68\, W / cm^2\right)$
- **Transient Control**



Temperature Contours
Re=2Pi, Pr=10

Dimensional Analysis

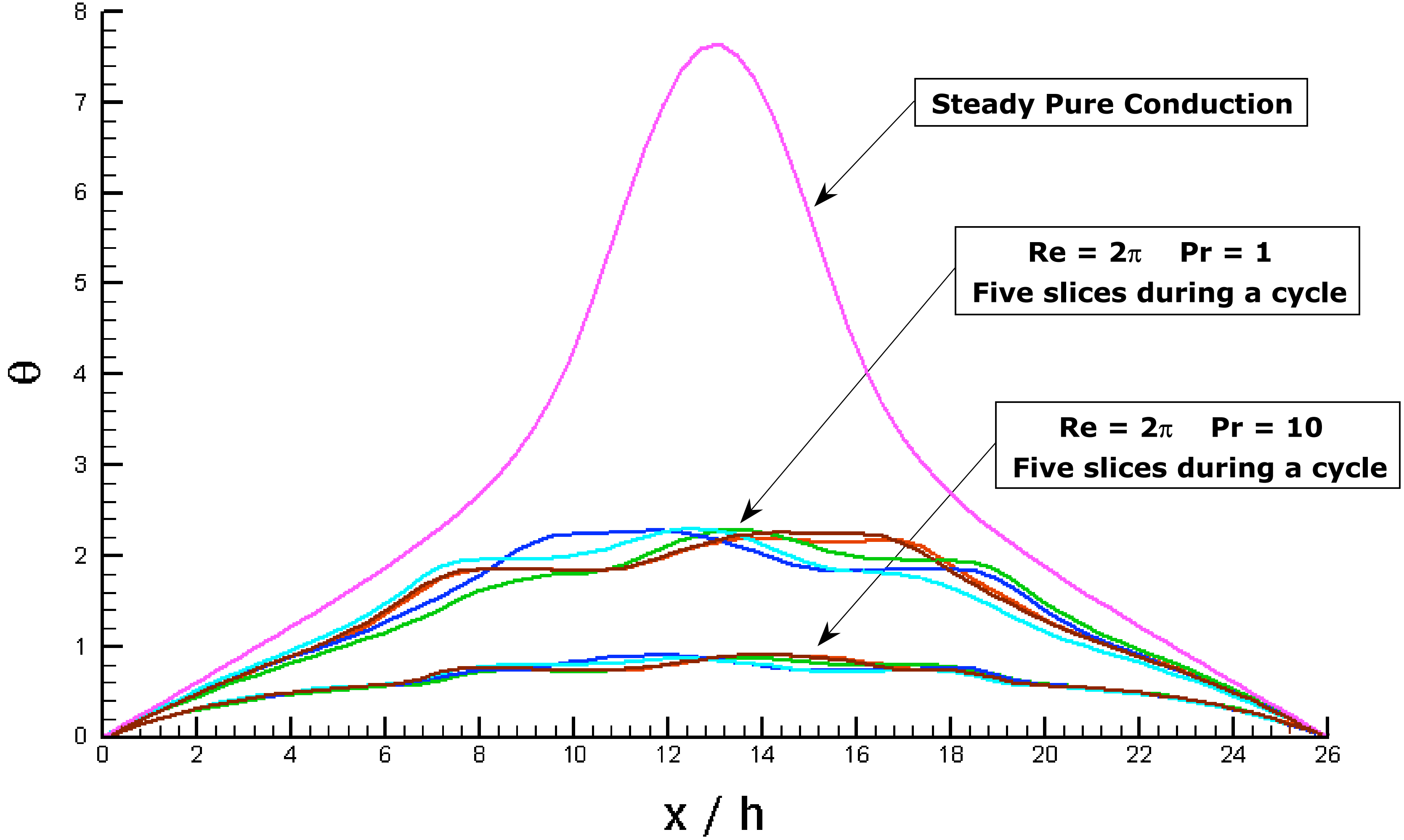
$$U_o = \omega a \qquad u^* = \frac{u}{U_o} \qquad v^* = \frac{v}{U_o}$$

$$Re = \frac{\omega a^2}{\nu} \qquad St = \frac{U_o}{\omega a} = 1 \qquad Pr = \frac{\mu C_p}{k}$$

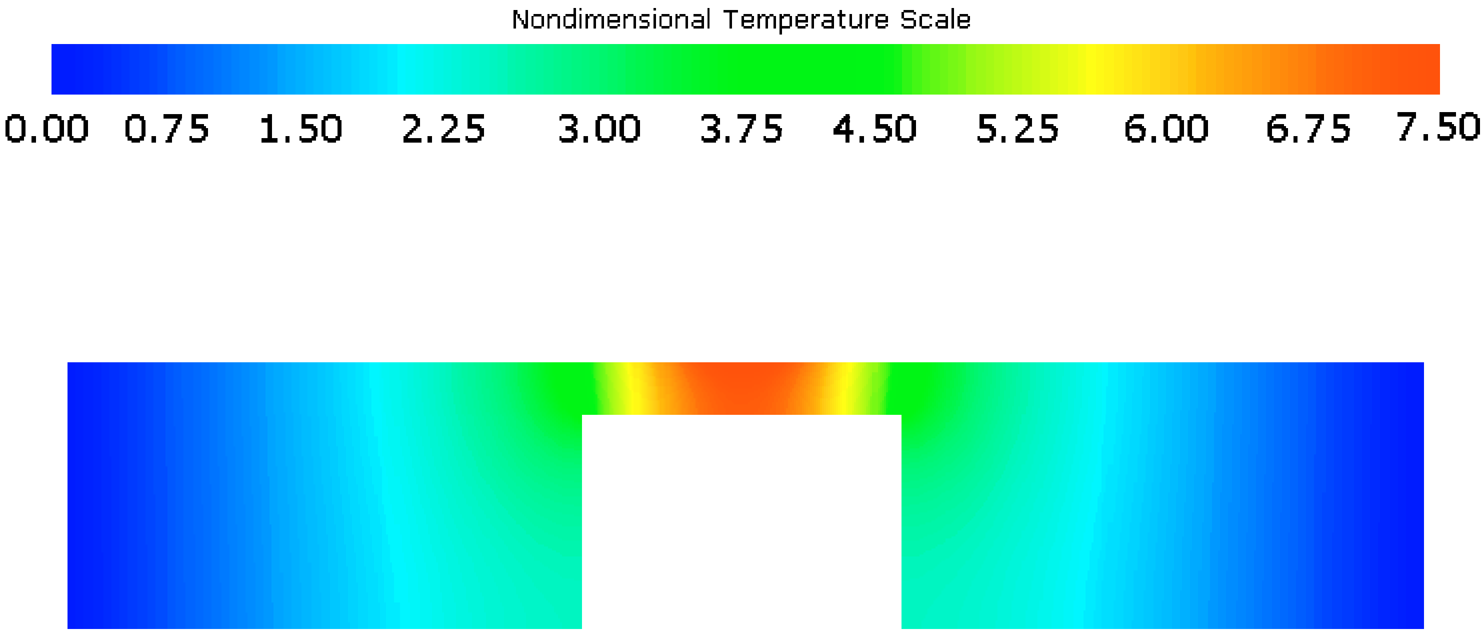
$$\theta = \frac{T - T_o}{\Delta T}$$

- Re & Pr are the only parameters.
- Simulations are done for
    - Re = 2π
    - Pr = 1 (~ air) & Pr = 10 (~ water)
- ΔT is a floating parameter.

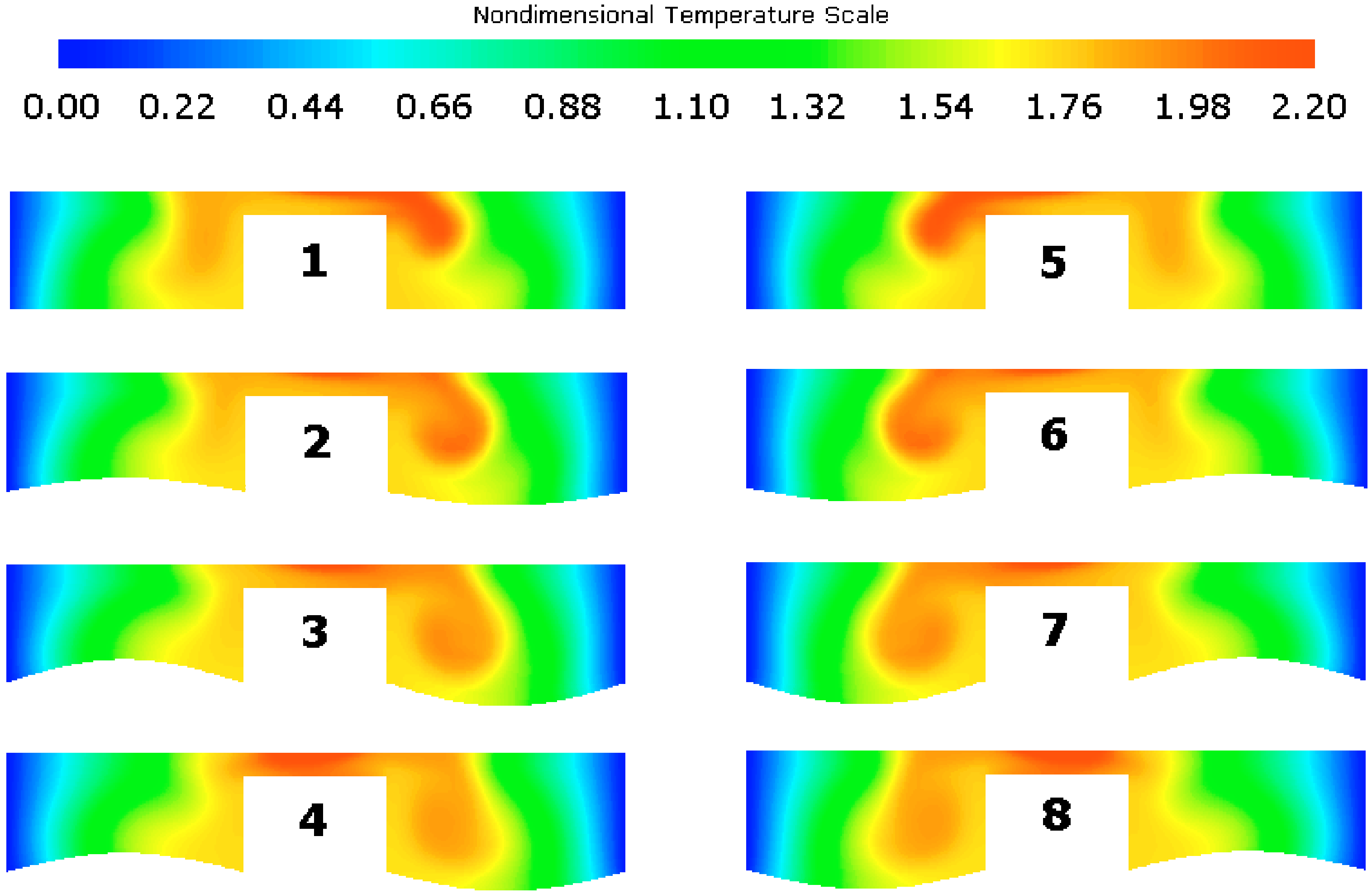
Nondimensional Temperature Distribution on the Surface of the MHS



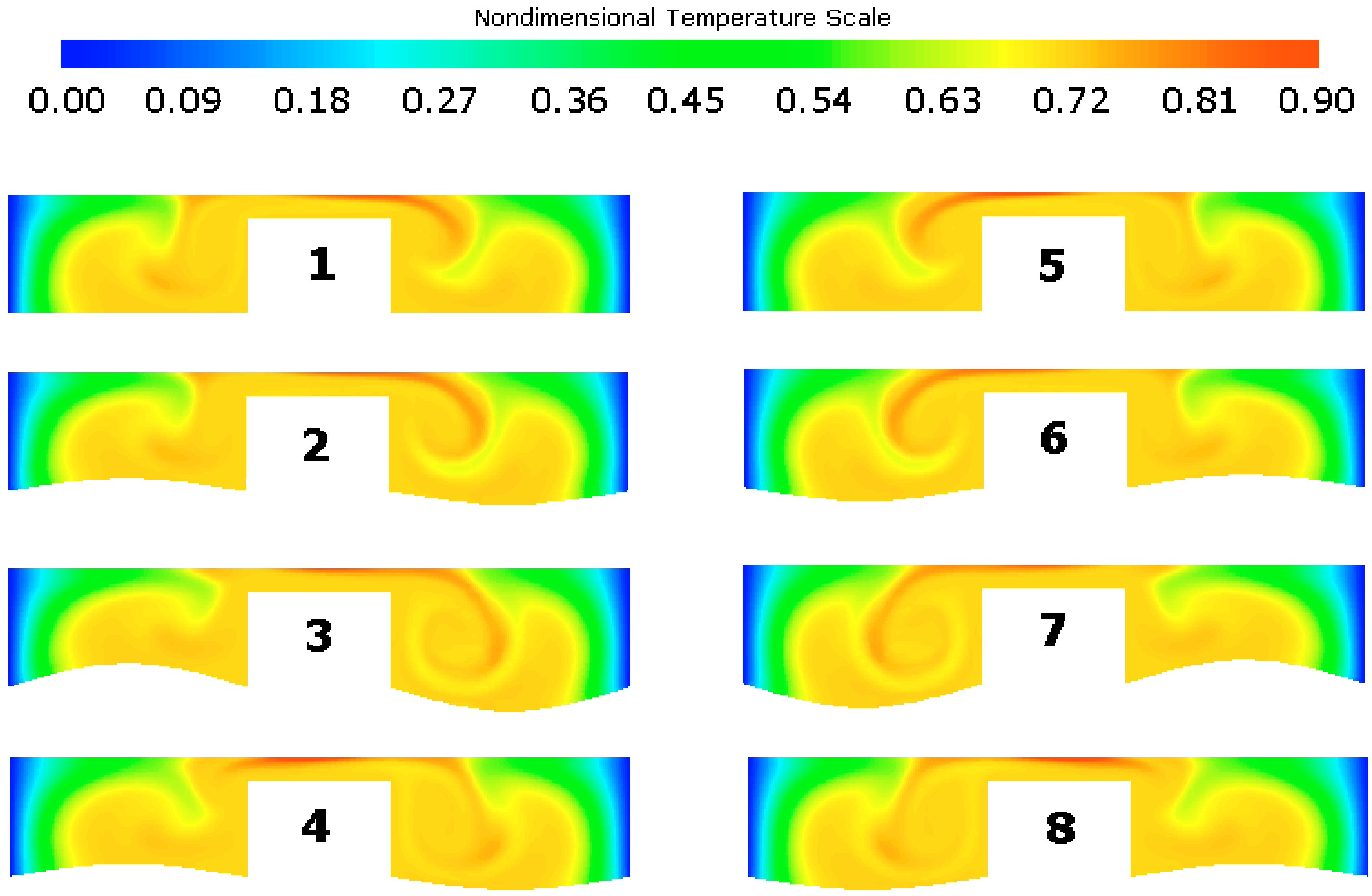
Pure Conduction



$Re = 2\pi$, $Pr = 1$ Snapshots



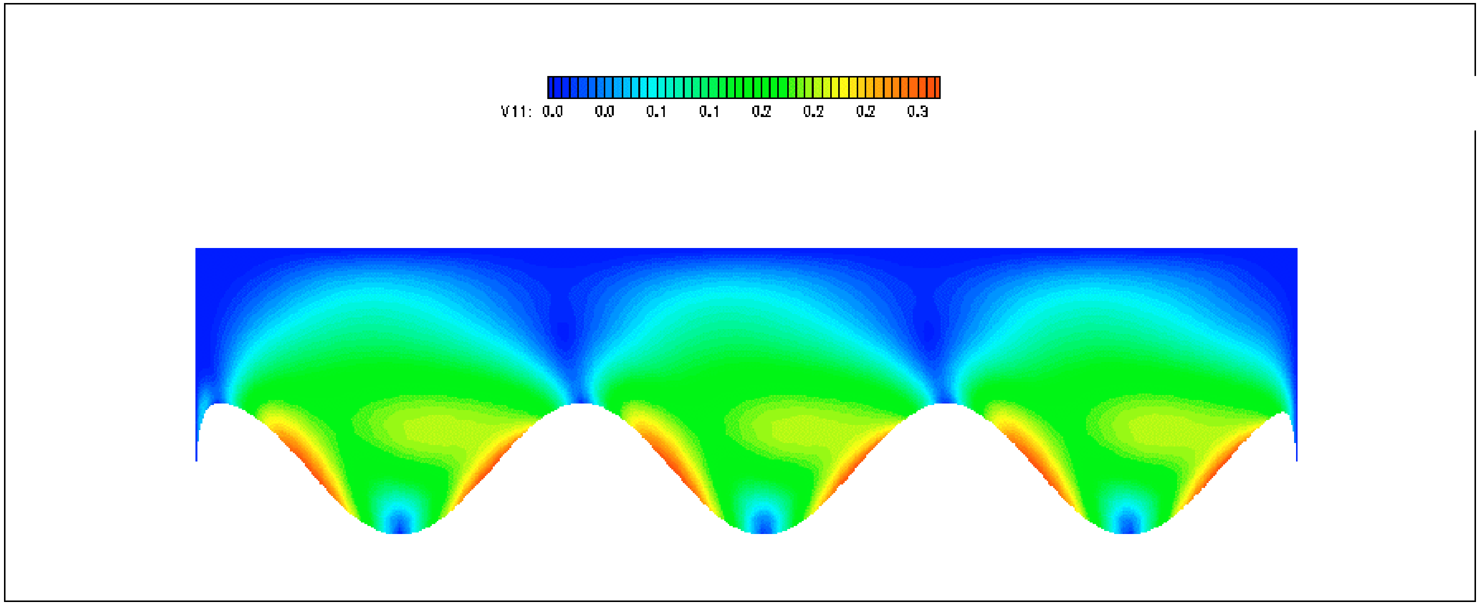
$Re = 2\pi$, $Pr = 10$ Snapshots



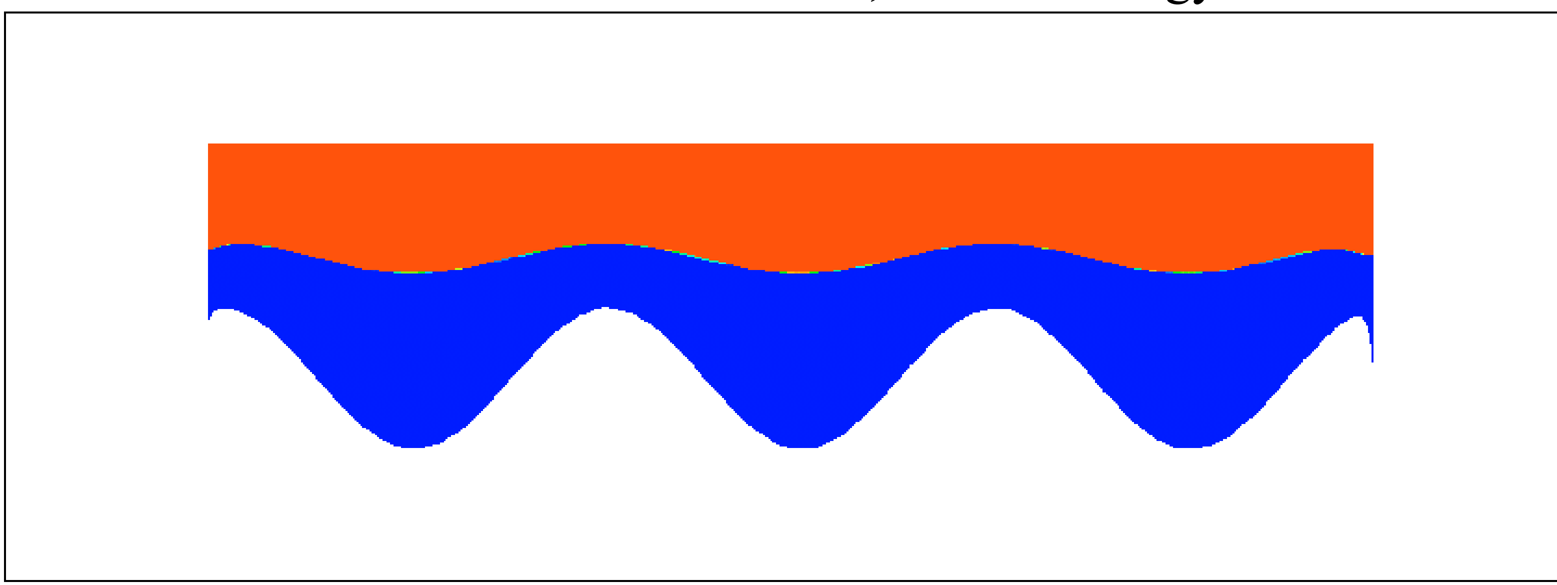
Micro Heat-Spreaders

- <u>Closed-loop single-phase</u> micro-fluidic systems.
- Actuated electrostatically.
- Based on <u>unsteady</u> forced convection in micro-channels.
- Achieve very high heat flux removal rates.
- Enable <u>active closed loop control</u> strategies.
- Are <u>MEMS</u> devices.
- Can be integrated to microchip design & fabrication.
- Heat dissipation to surrounding via the side walls with larger surface area enables conventional cooling strategies.

Chaotic Advection in a Peristaltic Micro-Mixer



Peristaltic Micro Mixer, Kinetic Energy



Peristaltic Micro Mixer, tracing an initially horizontal interface

Modeling Uncertainty

- Stochastically-excited structures
- Boundary conditions, geometry, properties
- Sensitivity/failure analysis
- Gaussian and non-Gaussian processes
- Polynomial Chaos vs. Monte Carlo
- Stochastic spectral/hp element methods

Uncertainties in MEMS

- Anisotropy in mechanical properties
- Polycrystalline silicon – random orientation/shapes of crystal grains
- First PhD (Mirfendereski, Berkeley'95) shows COV of 3% in response of micro-beams and 6% in frequency of lateral micro-resonators

Wiener, 1938; Ghanem & Spanos, 1991)

Representation of a Random Process

$$T(\mathbf{x},t;\theta)=\sum_{i=0}^{\infty}T_i(\mathbf{x},t)\Psi_i(\xi(\theta))$$

- $T(\mathbf{x},t;\theta)$ - Random process
  - $(\mathbf{x},t)$ - Spatial/temporal dimension
  - θ - Random dimension
- $T_i(\mathbf{x},t)$ - Deterministic coefficients
- $\Psi_i(\xi(\theta))$ - ***Generalized*** Polynomial Chaos

Generalized Polynomial Chaos

$$T(x,t;\theta) = \sum_{j=0}^{\infty} T_j(x,t)\Psi_j(\xi(\theta))$$

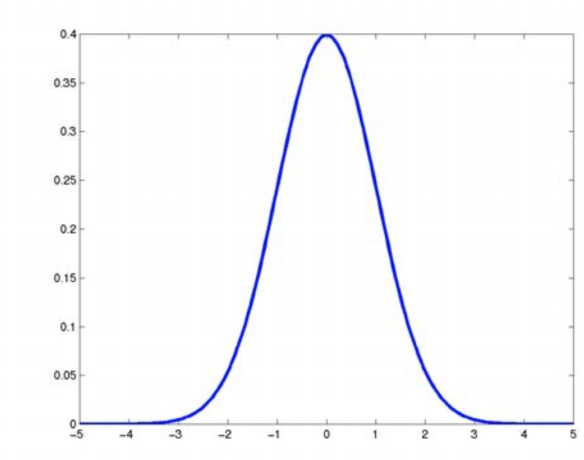
- Polynomials of random variable $\xi(\theta)$
- Orthogonality : $\langle \Psi_i \Psi_j \rangle = \langle \Psi_i^2 \rangle \delta_{ij}$

$$\langle f(\xi)g(\xi)\rangle = \int f(\xi)g(\xi)W(\xi)d\xi \quad \text{or} \quad \langle f(\xi)g(\xi)\rangle = \sum_i f(\xi_i)g(\xi_i)w(\xi_i)$$

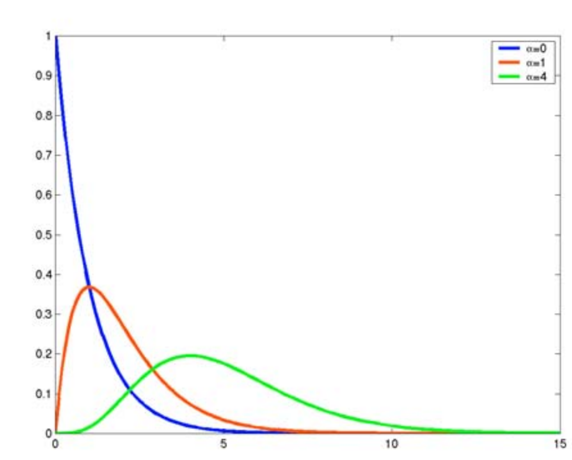
- Weight function determines underlying random variable (*not necessarily Gaussian*)
- Complete basis from *Askey scheme*
- Each set of basis converges in L^2 sense

Orthogonal Polynomials and Probability Distributions

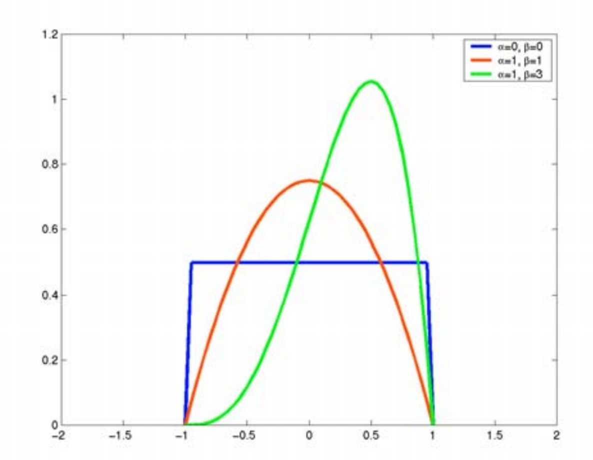
- **Continuous Cases**:
  - *Hermite* Polynomials ⟷ *Gaussian* Distribution
  - *Laguerre* Polynomials ⟷ *Gamma* Distribution (special case: *exponential* distribution)
  - *Jacobi* Polynomials ⟷ *Beta* Distribution
  - *Legendre* Polynomials ⟷ *Uniform* Distribution



Gaussian distribution



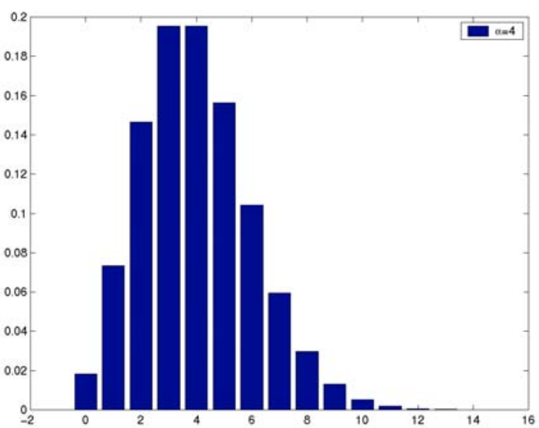
Gamma distribution



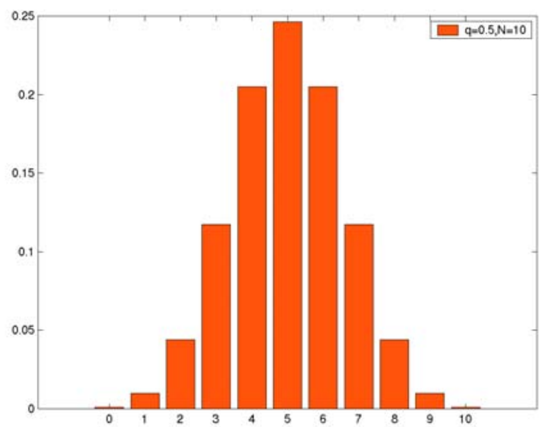
Beta distribution

Orthogonal Polynomials and Probability Distributions

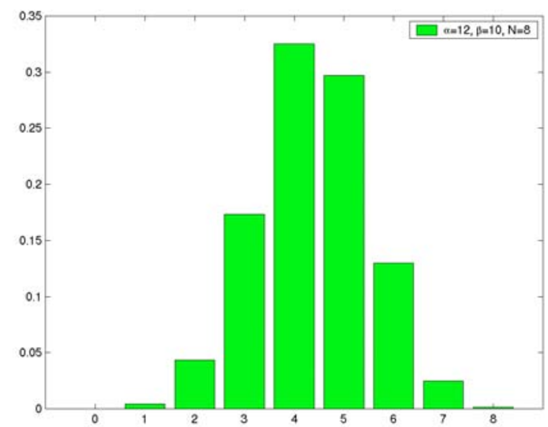
- **Discrete Cases :**
  - *Charlier* Polynomials ⟷ *Poisson* Distribution
  - *Krawtchouk* Polynomials ⟷ *Binomial* Distribution
  - *Hahn* Polynomials ⟷ *Hypergeometric* Distribution
  - *Meixner* Polynomials ⟷ *Pascal* Distribution



Poisson distribution



Binomial distribution



Hypergeometric distribution

Applications : ODE with Uncertain Coefficients

- Equation : $$\frac{dy}{dt} = -ky, \quad y\big|_{t=0} = \hat{y}.$$

k is the decaying coefficient with given probability distribution.

- Chaos expansion :

$$y(x,t;\theta) = \sum_{i=0}^{P} y_i(x,t)\Psi_i(\xi(\theta)), \quad k(\theta) = \sum_{i=0}^{P} k_i \Psi_i(\xi(\theta))$$

- Galerkin projection :

$$\frac{dy_i}{dt} = -\frac{1}{\langle \Psi_k^2 \rangle} \sum_{i=0}^{P} \sum_{j=0}^{P} \langle \Psi_i \Psi_j \Psi_k \rangle k_i y_j, \quad k = 0, 1, 2, \ldots, P$$

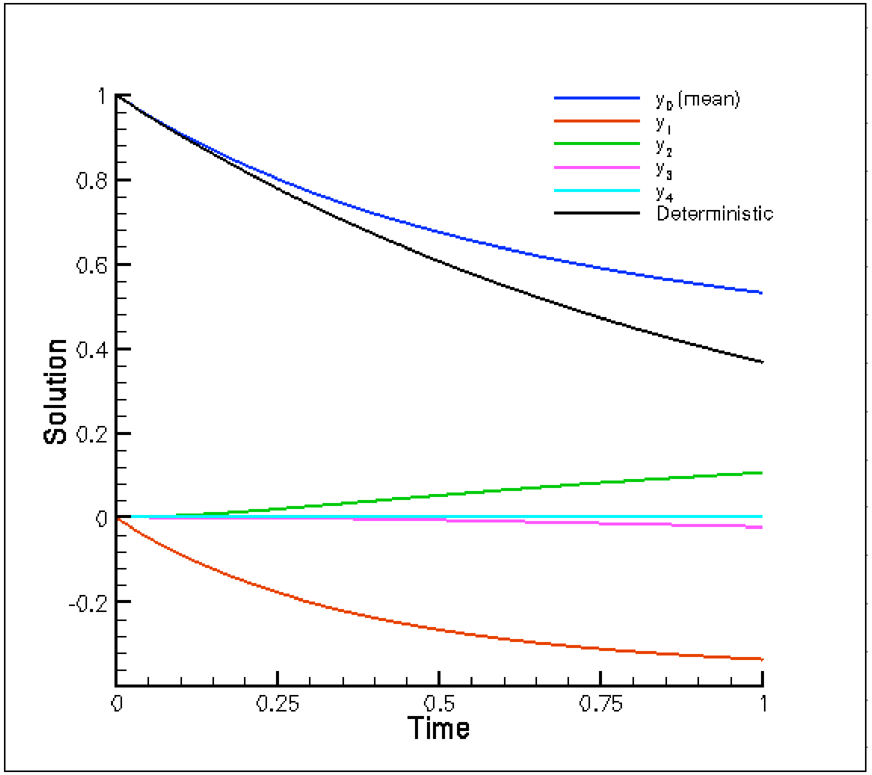
- The Chaos will be chosen according to the distribution of *k*.

- L^{inf} error : $$\left| \frac{\bar{y}_{chaos}(t) - \bar{y}_{exact}(t)}{\bar{y}_{exact}(t)} \right|$$

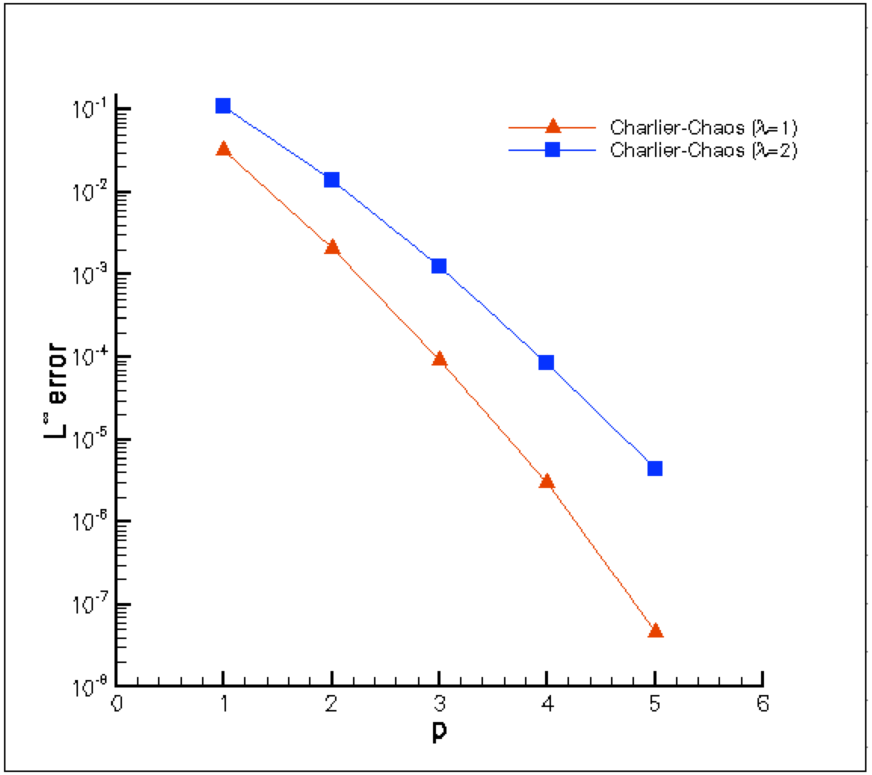
Discrete Distribution : Poisson (Charlier-Chaos)

- $dy/dt = -k\,y,\ \ y(t=0)=1$
- k is a **Poisson** random variable :

$$\text{PDF}:\ \ f_k(x) = e^{-\lambda}\frac{\lambda^x}{x!},\ \ x = 0, 1, 2, \ldots$$



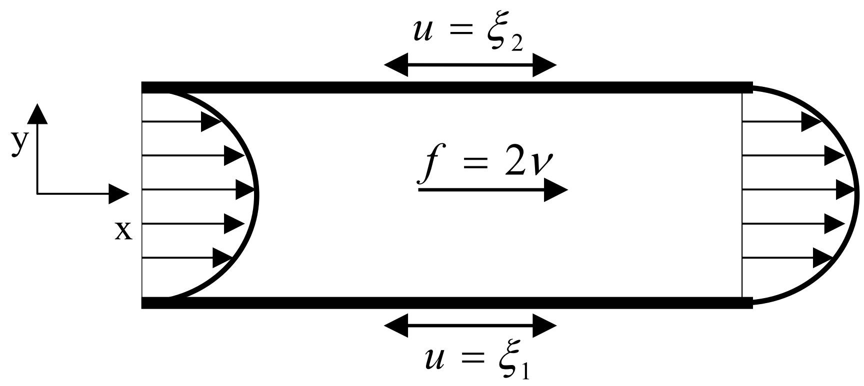
Solution of expansion modes : $\lambda = 1$



Convergence w.r.t. expansion terms

- 4^{th}-order **Charlier-Chaos** expansion
- Exponential convergence rate

Channel flow with Random Boundary Conditions

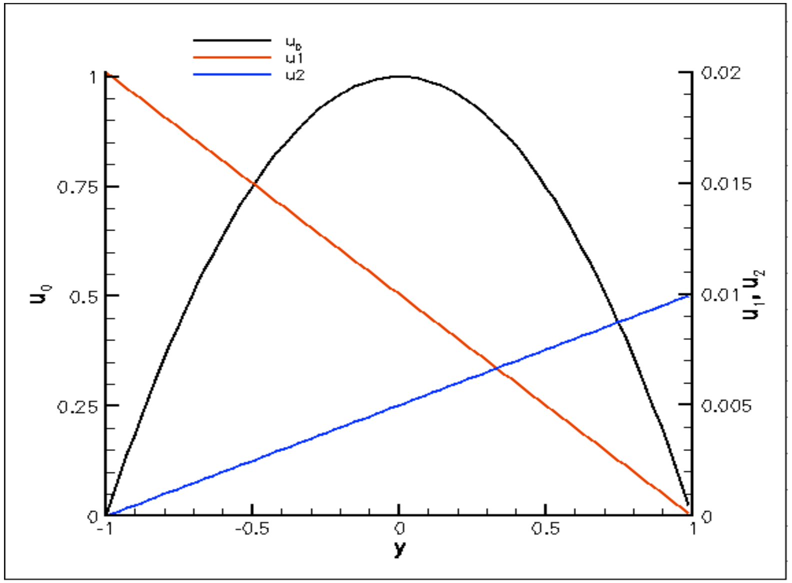


Exact solution (uniform BCs):

$$u(y) = (1 - y^2) + \frac{1-y}{2}\sigma_1\xi_1 + \frac{1+y}{2}\sigma_2\xi_2$$

- Two-dimensional PC expansion
- Gaussian inputs :

$$\sigma_1 = 2\%, \quad \sigma_2 = 1\%$$



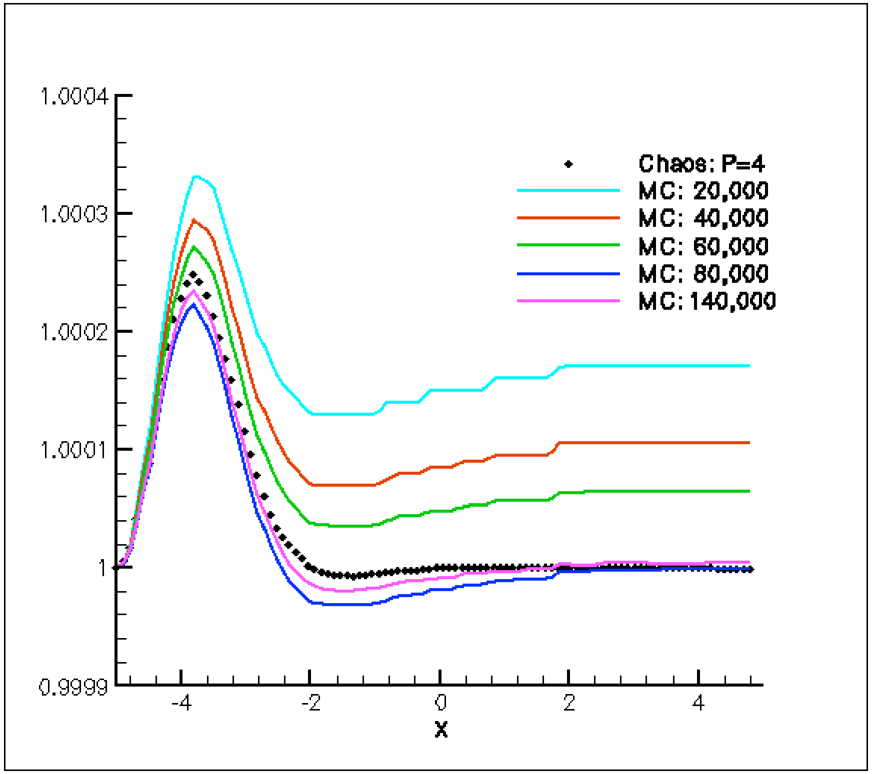
Solution profile across the channel

Non-uniform Exponential Random BC

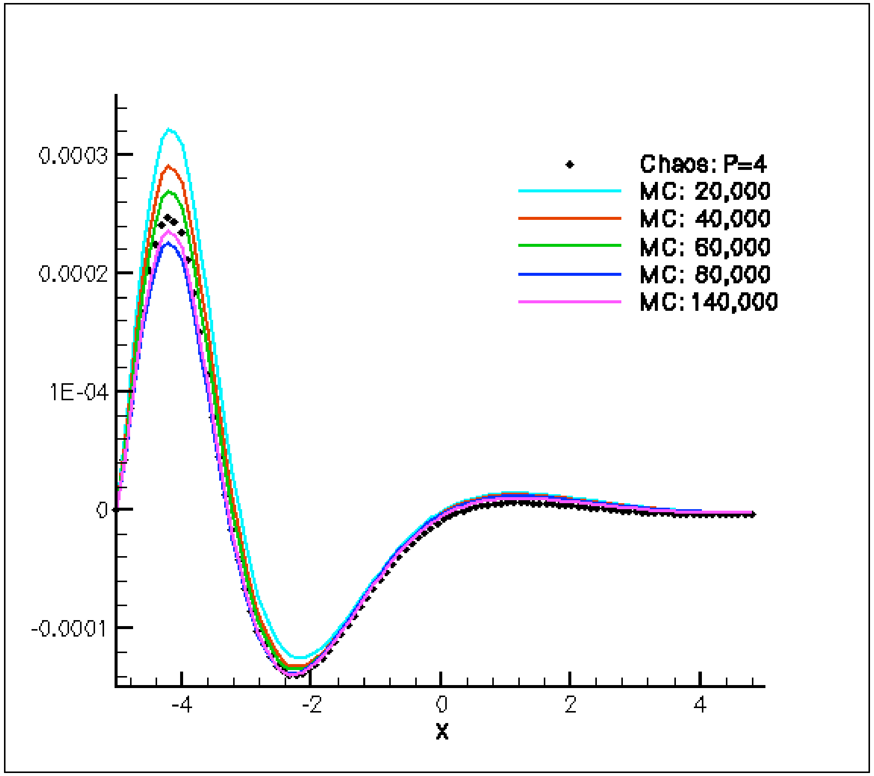
- Exponential correlation

$$C(x_1, x_2) = \sigma^2 e^{-|x_1 - x_2|/b}$$

- Stochastic input: $\sigma = 0.1$
- 2D K-L expansion
- 4th-order Laguerre-Chaos expansion
- 15-term expansion

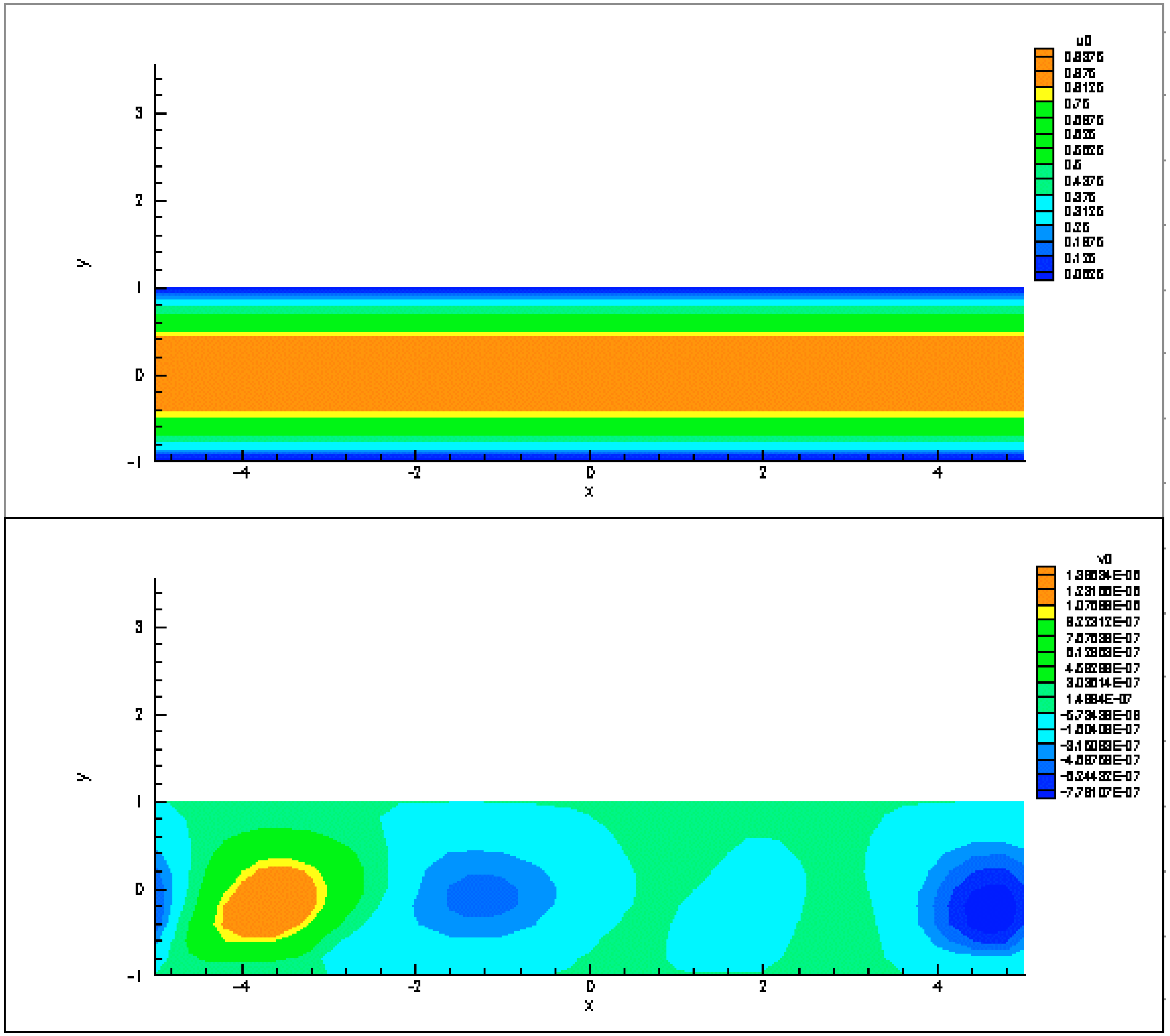


U_{mean} along centerline

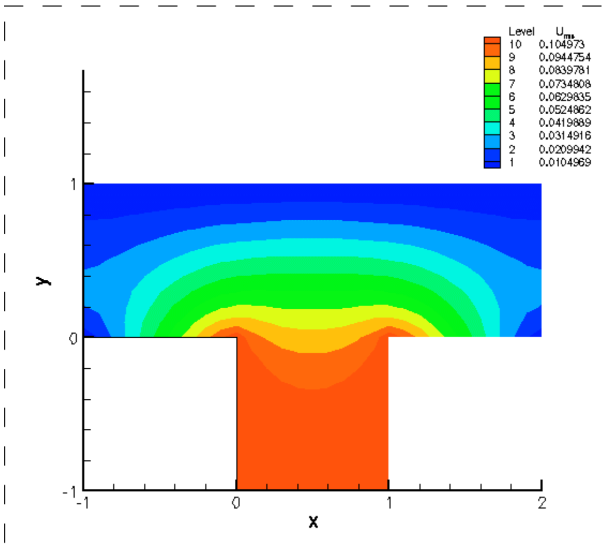


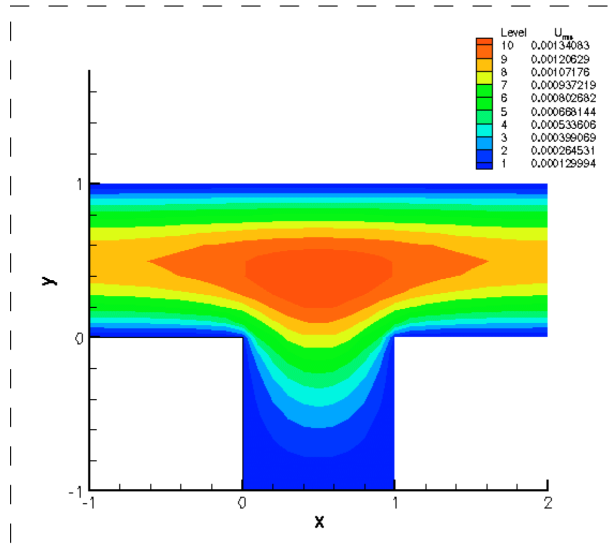
V_{mean} along centerline

Non-Uniform Uncertainty at Wall



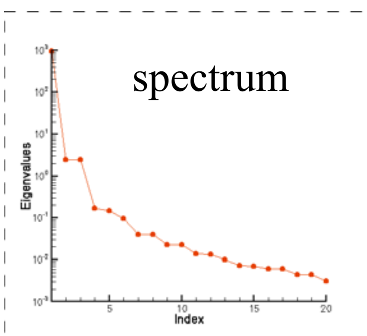
Heat Transfer in a Microcavity: Noisy B.C. versus Noisy Conductivity

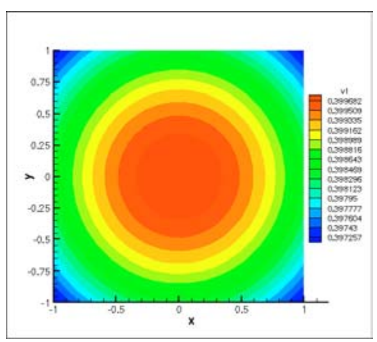




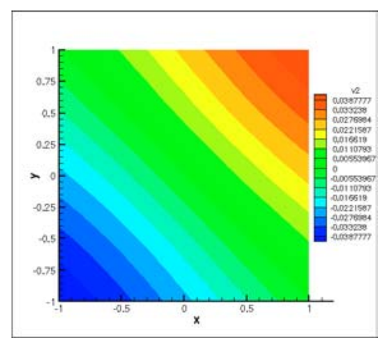
* Stochastic B.C.

* Stochastic conductivity





KL-1



KL-2