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Biofilm Characterization using Large Scale Optimization

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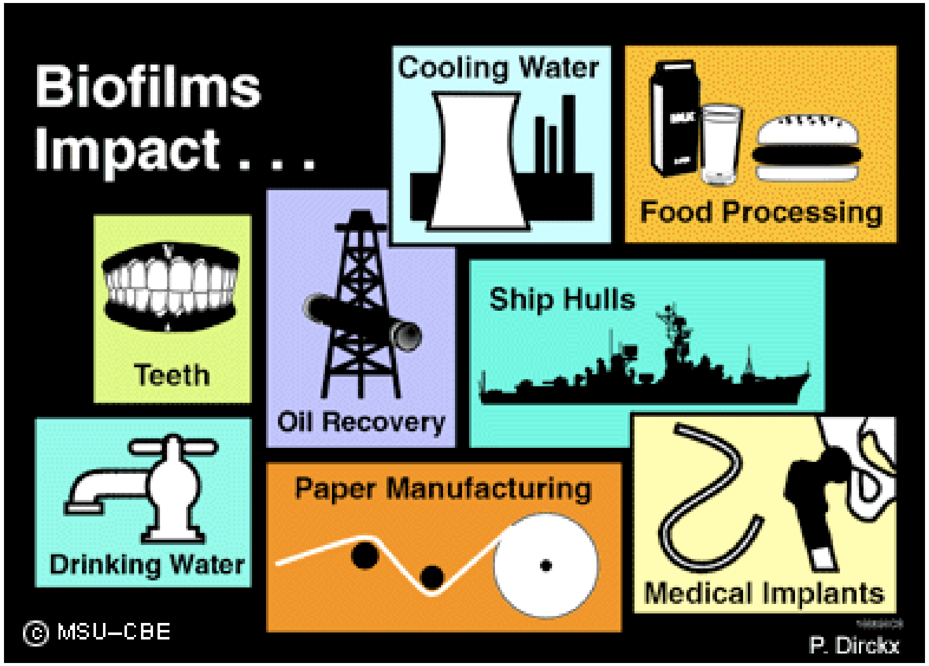
Motivation: Definition and Impact

A biofilm is a complex aggregation of microorganisms marked by the excretion of a protective and adhesive matrix.



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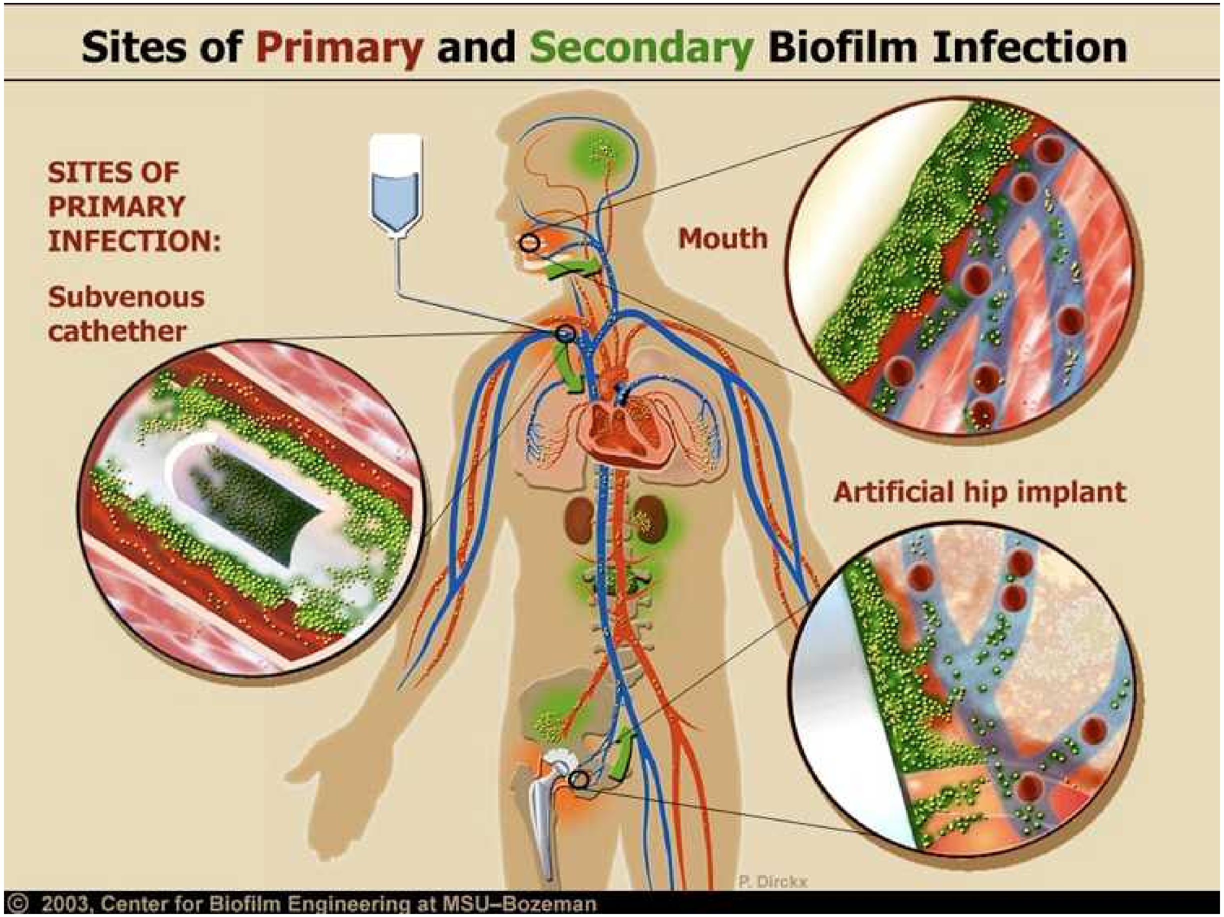
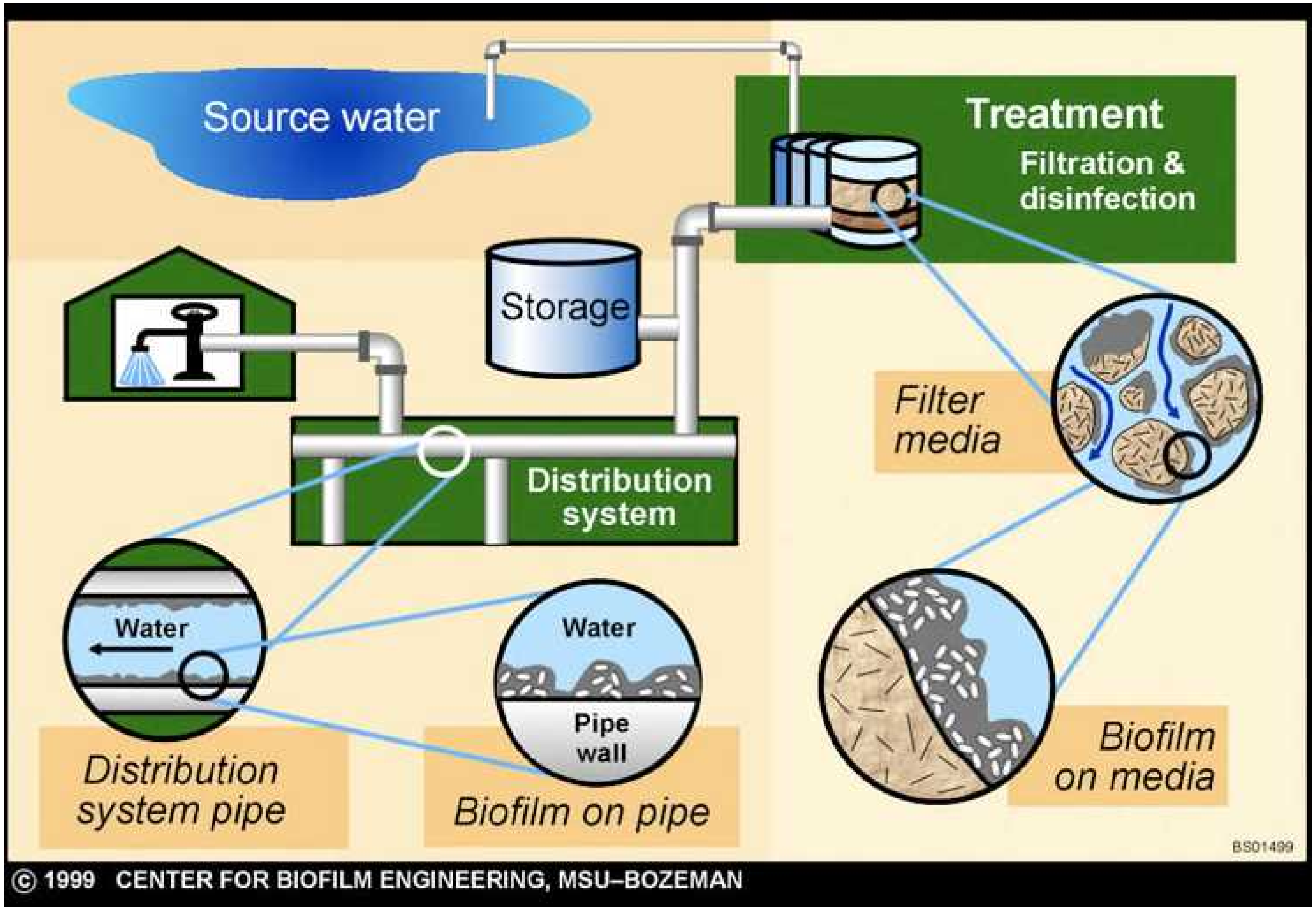
Motivation: Human Physiology



Motivation: Water Distribution & Security



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Goals of the project:

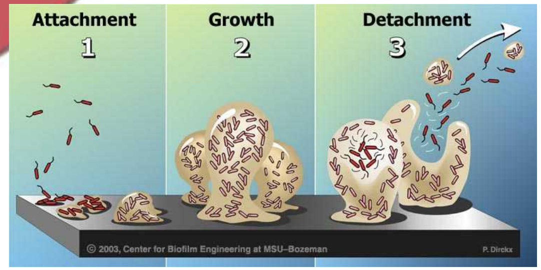
- Develop simulation capabilities to predict the dynamics of biofilms
- Calibrate model with experimental observations
- Develop efficient and flexible extension capabilities
- Characterize uncertainties

Outline

- Motivation
- Physics
- Inversion
- Implementation
- Numerical examples/results

Goal of the presentation: 1) motivate **PDE C**onstrained **O**ptimization through biofilm problem, 2) demonstrate convenient PDECO framework

- Bacteria Adhesion
- EPS Production
- Bacteria duplication
- Transport of interface
- Detachment



Biofilm Physics

Multi-species Model for growth:

(Alpkvist and Klapper 06)

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Simplified model:

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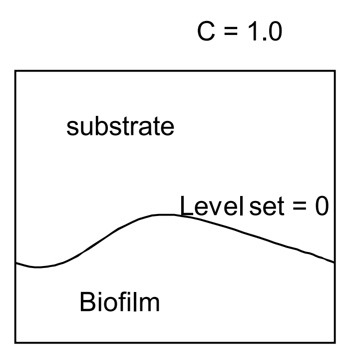
TIFF (Uncompressed) decompressor
are needed to see this picture.

Computational domain:

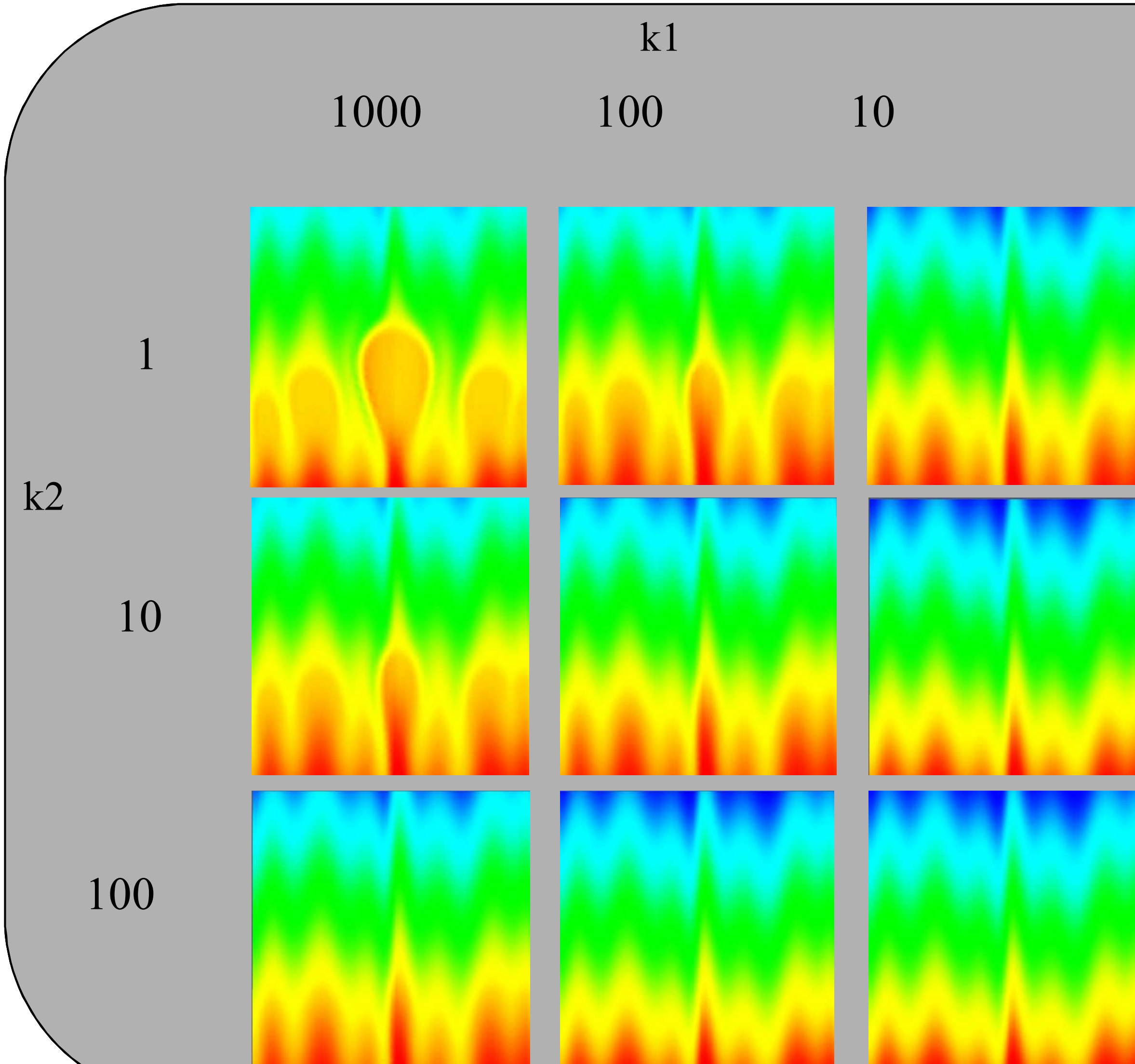


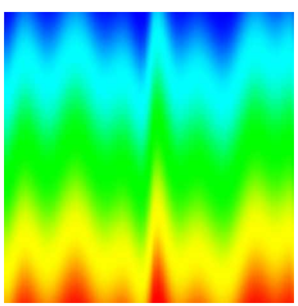
Forward Simulation Results
(Realizations shown at final timestep)

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

<u>Simulation Details</u>:

- deltaT = 0.005
- grid 64x64
- D = 1.0
- Newton-GMRES
- ILU preconditioner
- CPU time = 70s





Initial Condition

Forward Simulation Results

(Realizations shown at final timestep)

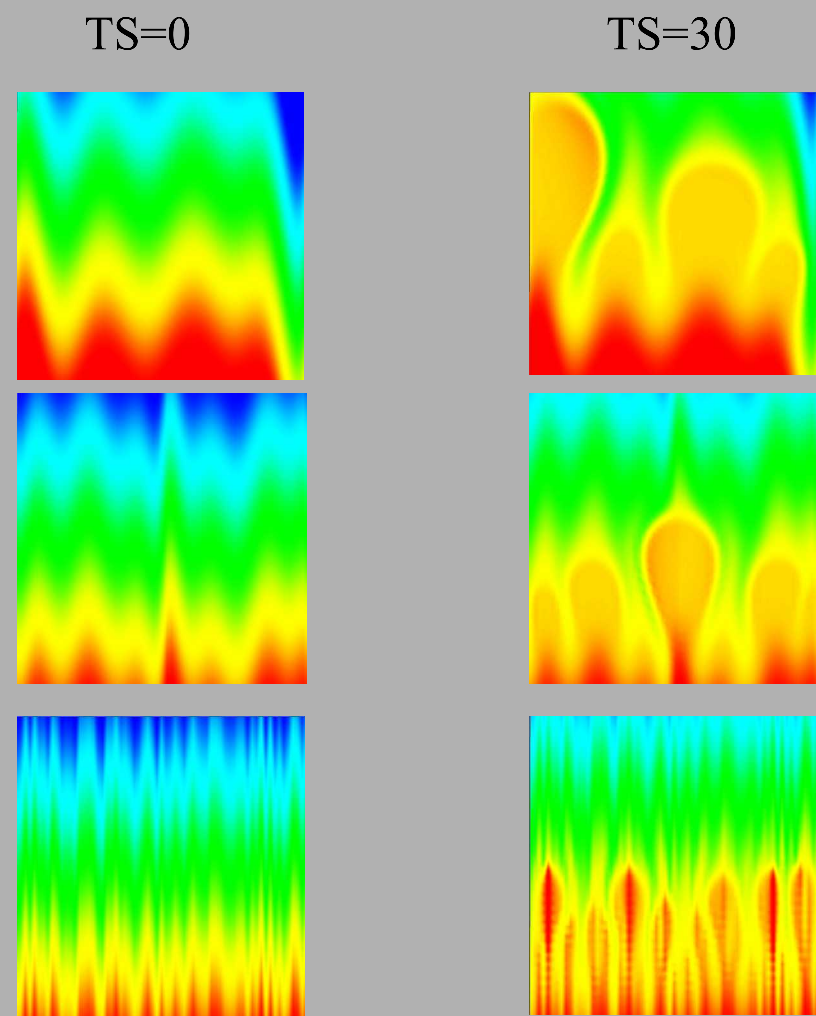
QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Simulation Details:

- timesteps = 30
- deltaT = 0.005
- grid 64x64
- D = 1.0
- Newton-GMRES
- ILU preconditioner
- CPU time = 70s

Constant:

- K1 = 1000.0
- K2 = 1.0



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Biofilm Optimization Formulation

The PDE constrained optimization problem

$$\min_{\rho,\rho_o} \; \mathcal{F}(\rho,\rho_u) = \frac{1}{2}\sum_{i=0}^{N}\int_0^T \int_\Omega (\rho-\rho^*)^2\delta(x-x_i)\,\mathbf{dx}\,\mathbf{dt} + \frac{\beta}{\mathbf{2}}\int_{\mathbf{\Omega}} \rho_{\mathbf{0}}^{\mathbf{2}}\,\mathbf{dx}$$

subject to:

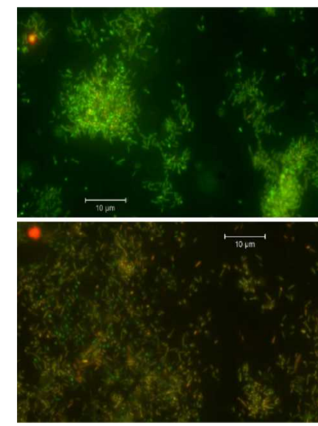
$$\frac{\partial\rho}{\partial t} + \frac{D}{\rho_b}\nabla c\cdot\nabla\rho = 0 \qquad \text{in} \quad \Omega\times[0,T]$$

$$\rho = \rho_0 \qquad \text{in} \quad \Omega\times\{t=0\}.$$

$$D\Delta c = \frac{k_1 c\rho}{k_2 + c} \qquad \text{in} \quad \Omega$$

$$c = c_D \qquad \text{in} \quad \Gamma_D$$

Match confocal microscope images



Biofilm Optimality Conditions

The forward coupled problem

$$D\Delta c = \frac{k_1 c\rho}{k_2 + c} \quad \text{in } \Omega$$

$$c = c_D \quad \text{in } \Gamma_D$$

$$\frac{\partial \rho}{\partial t} + \frac{D}{\rho_b}\nabla c \cdot \nabla \rho = 0 \quad \text{in } \Omega \times [0, T]$$

$$\rho = \rho_0 \quad \text{in } \Omega \times \{t = 0\}.$$

The adjoint problem

$$D\Delta\lambda_1 - \frac{k_1 k_2 \rho}{(k_2 + c)^2}\lambda_1 - \frac{D}{\rho_b}\lambda_2 \Delta\rho = 0 \quad \text{in } \Omega$$

$$-D\nabla\lambda_1 \cdot n + \lambda_2 \frac{D}{\rho_b}\nabla\rho \cdot n = 0 \quad \text{on } \Gamma_N$$

$$\lambda_1 = 0 \quad \text{on } \Gamma_D$$

$$-\frac{\partial \lambda_2}{\partial t} - \frac{D}{\rho_b}\lambda_2 \Delta c - \frac{k_1 c \lambda_1}{k_2 + c} = -\Sigma(\rho - \rho^*)\delta_j \quad \text{in } \Omega \times [0, T]$$

$$\lambda_2 = 0 \quad \text{in } \Omega \times \{t = 0\}$$

The initial concentration equation

$$\beta\,\rho_0 - \lambda_2|_{t=0} = 0 \quad \text{in } \Omega.$$

Implementation Goals

Need **efficient** capability to implement **embedded** algorithms (i.e. PDECO)

Possible solutions: compile time transformation (**tricky** on complex codes), friendly interfaces, i.e. Comsol (**slow, inflexible**), armies of programmers (**expensive, error-prone, unmaintainable**

Our approach: 1) State in **mathematical form** the general problem of "writing" an efficient intrusive code 2) Write (**by hand**) a code to solve that meta-problem, 3) Write papers while the computer does the dirty work

Added benefits: The key to intrusion turns out to **simplify automation** as well a mathematical definition of the simulation development process aids in establishing **code correctness**

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Implementation Mathematics

- Test/Unkown/Auxiliary variables
- Functional spaces
- Frechet differentiation
- Discrete spaces

Examples:

Steady Navier-Stokes flow

$$F[\mathbf{v},\mathbf{u},q,p] = \int_\Omega [\nu \nabla \mathbf{v} : \nabla \mathbf{u} + p \nabla \cdot \mathbf{v} + \mathbf{v} \cdot (\mathbf{u} \cdot \nabla) \mathbf{u} + q \nabla \cdot \mathbf{u}]$$

Lagrangian for Poisson source inversion w/ Tikhonov

$$F[v,\mu,\beta,u,\lambda,\alpha] = \int_\Omega [(u-u^*)\, v + \nabla\lambda \cdot \nabla v]\, dx + \\ + \int_\Omega [\nabla\mu \cdot \nabla u + \mu\alpha]\, dx + \\ + \int_\Omega [\nabla\alpha \cdot \nabla\beta + \lambda\beta]\, dx$$

Approach unifies diverse set of problems:

A linearized forward problem: find Newton step $\delta\mathbf{u}$ at $\mathbf{u}_0$

$$\left.\frac{\partial \hat{F}}{\partial v_i}\right|_{\mathbf{u}_0} + \left.\frac{\partial^2 \hat{F}}{\partial v_i \partial u_j}\right|_{\mathbf{u}_0} \delta u_j = 0$$

A quadratic eigensystem: find σ, $\mathbf{u}$

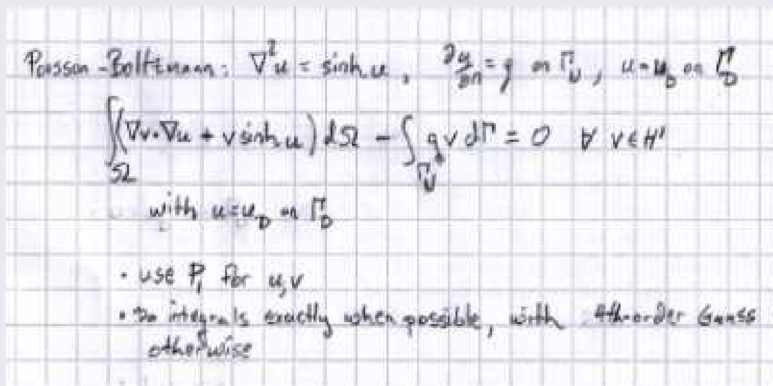
$$\left.\frac{\partial^2 \hat{F}}{\partial v_i \partial u_j}\right|_0 u_j + \left.\frac{\partial^3 \hat{F}}{\partial v_i \partial u_j \partial \sigma}\right|_0 \sigma u_j + \frac{1}{2} \left.\frac{\partial^4 \hat{F}}{\partial v_i\, \partial u_j\, \partial \sigma^2}\right|_0 u_j \sigma^2 = 0$$

A sensitivity problem: find $\partial\mathbf{u}/\partial\sigma$ at $\mathbf{u}_0$

$$\left.\frac{\partial^2 \hat{F}}{\partial v_i\, \partial \sigma}\right|_{\mathbf{u}_0} + \left.\frac{\partial^2 \hat{F}}{\partial v_i\, \partial u_j}\right|_{\mathbf{u}_0} \frac{\partial u_j}{\partial \sigma} = 0$$

Implementation Syntax

Sundance is a toolkit that is based on these principles



Poisson-Boltzmann: $\nabla^2 u = \sinh u$, $\frac{\partial u}{\partial n} = g$ on Γ_N, $u = u_D$ on Γ_D

$$\int_\Omega (\nabla v \cdot \nabla u + v \sinh u)\, d\Omega - \int_{\Gamma_N} g v \, d\Gamma = 0 \quad \forall\, v \in H^1$$

with $u = u_D$ on Γ_D

- use P_1 for u, v
- Do integrals exactly when possible, with 4th-order Gauss otherwise

Poisson-Boltzmann equation in a notebook

```
u = UnknownFunction(Lagrange(1))
v = TestFunction(Lagrange(1))

quad = GaussianQuadrature(4)

weak = Integral(omega,(grad*u)*(grad*v)+v*sinh(u), quad)
```

Poisson-Boltzmann equation in Sundance

Implementation Syntax for Optimization: Approach 1

The forward coupled problem

$$
\begin{aligned}
D\Delta c &= \frac{k_1 c\rho}{k_2+c} && \text{in } \Omega\\
c &= c_D && \text{in } \Gamma_D\\
\frac{\partial\rho}{\partial t} + \frac{D}{\rho_b}\nabla c\cdot\nabla\rho &= 0 && \text{in } \Omega\times[0,T]\\
\rho &= \rho_0 && \text{in } \Omega\times\{t=0\}.
\end{aligned}
$$

The adjoint problem

$$
\begin{aligned}
D\Delta\lambda_1 - \frac{k_1k_2\rho}{(k_2+c)^2}\lambda_1 - \frac{D}{\rho_b}\lambda_2\Delta\rho &= 0 && \text{in } \Omega\\
-D\nabla\lambda_1\cdot n + \lambda_2\frac{D}{\rho_b}\nabla\rho\cdot n &= 0 && \text{on } \Gamma_N\\
\lambda_1 &= 0 && \text{on } \Gamma_D\\
-\frac{\partial\lambda_2}{\partial t} - \frac{D}{\rho_b}\lambda_2\Delta c - \frac{k_1 c\lambda_1}{k_2+c} &= -\Sigma(\rho-\rho^*)\delta_j && \text{in } \Omega\times[0,T]\\
\lambda_2 &= 0 && \text{in } \Omega\times\{t=0\}
\end{aligned}
$$

The initial concentration equation

$$\beta\,\rho_0 - \lambda_2|_{t=0} = 0 \qquad \text{in } \Omega.$$

forward

```
Expr state = Integral(interior, (u - u0)*uHat* 1.0/deltaT + v*(grad*u)*uHat
                                + D*(grad*uHat)*(grad*u), q2);
Expr stateBC = EssentialBC(left, u*uHat, q2);

stateProb = rcp(new LinearProblem(mesh_, state, stateBC, mu, u, vecType));
```

adjoint

```
CellFilter sensors = sensorFilter() ;

Expr adjoint = Integral(interior, (lambda - lambda0)*v/deltaT
                                    + D*(grad*u)*(grad*lambda)
                                    + v*(grad*u)*lambda, q2)
                                    + Integral(sensors, v*(u - uTarget), q2) ;

Expr adjointBC = EssentialBC(left, lambda*v, q2)
               + EssentialBC(bottom, lambda*v, q2) ;

adjointProb = rcp(new LinearProblem(mesh_, adjoint, adjointBC,
                                     v, lambda, vecType));
```

sensitivity

```
Expr sens = Integral(interior_, -Reg_ * u0_*beta + lambda0_*beta + beta*u, q2);

Expr sensBC;
Expr sensProb = new LinearProblem(mesh, sens, sensBC, beta, u, vecType);
```

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Implementation Syntax for Optimization: Approach 2

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TIFF (Uncompressed) decompressor
are needed to see this picture.

```
Expr lag = Integral(interior, 0.5*pow(u - target, 2.0) *direcDelta + R*alpha*alpha
                    + (u - uOld)*lambda + deltaT*D*(grad*lambda)*(grad*u)
                    + lambda*v*(grad * u), q2);
```

Lagrangian definition

```
Expr lagBC = EssentialBC(left, lambda*u, q2);
```

Boundary conditions

```
Functional L(mesh, lag, lagBC, vecType);
LinearProblem stateProb = L.linearVariationalProb(lambda, lambda0,
                                                  u, alpha, alpha0);
```

Define functional

Variational statement

```
LinearSolver<double> solver
  = LinearSolverBuilder::createSolver(solverParams);
```

Solver definition

```
  for (int i=0; i<Nts; i++)
 {

  uSoln = stateProb.solve(solver);
  CopyOldSol(uSoln, uOld);

 }
```

Time-stepping loop

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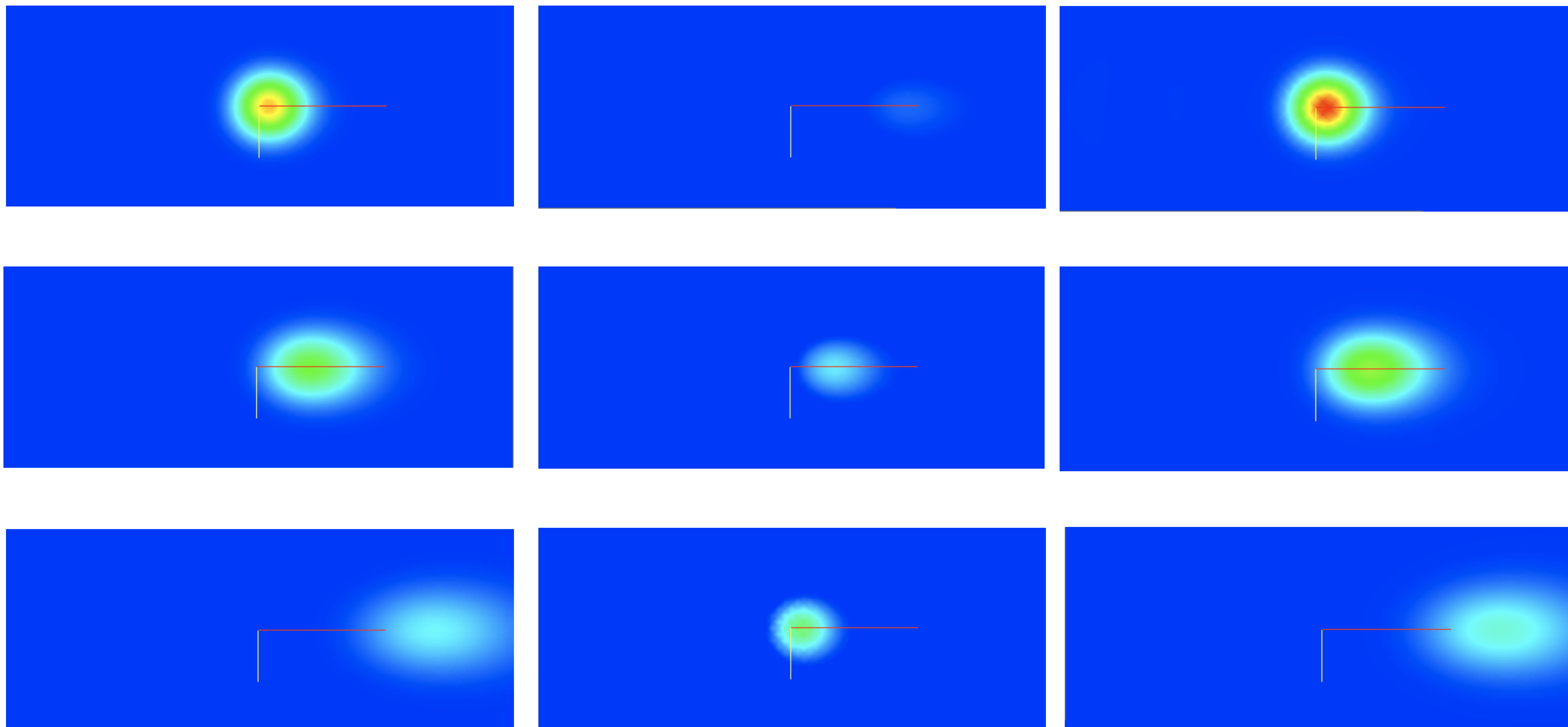
Example: Convection Diffusion Forward and Adjoint

Target : Adjoint : Inversion:



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Biofilm Inversion Formulation and implementation
Approach 1

The PDE constrained optimization problem

$$\min_{\rho,\rho_o} \mathcal{F}(\rho,\rho_u) = \frac{1}{2}\sum_{i=0}^{N}\int_0^T \int_\Omega (\rho-\rho^*)^2\delta(x-x_i)\,\mathbf{dx}\,\mathbf{dt} + \frac{\beta}{\mathbf{2}}\int_\Omega \rho_0^2\,\mathbf{dx}$$

subject to:

$$\begin{aligned} \frac{\partial\rho}{\partial t} + \frac{D}{\rho_b}\nabla c\cdot\nabla\rho &= 0 && \text{in } \Omega\times[0,T] \\ \rho &= \rho_0 && \text{in } \Omega\times\{t=0\}. \\ D\Delta c &= \frac{k_1 c\rho}{k_2+c} && \text{in } \Omega \\ c &= c_D && \text{in } \Gamma_D \end{aligned}$$

Additional complications:

- SUPG
- Crank-Nicholson

```
Expr state = Integral(interior_, (rho - rho0_)*rhoHat/deltaT
                                 +0.5*(D_/rhoB_)*((grad*rho)*(grad*c))*rhoHat
                                 +0.5*(D_/rhoB_)*((grad*rho0_)*(grad*c0_))*rhoHat

                                 +(rho - rho0_)/deltaT
                                   *stau*(D_/rhoB_)*((grad*st2)*(grad*rhoHat))
                                 +0.5*(D_/rhoB_)*((grad*rho)*(grad*c))*rhoHat
                                   *stau*(D_/rhoB_)*((grad*st2)*(grad*rhoHat))
                                 +0.5*(D_/rhoB_)*((grad*rho0_)*(grad*c0_))*rhoHat
                                   *stau*(D_/rhoB_)*((grad*st2)*(grad*rhoHat))

                                 -D_*(grad*c)*(grad*cHat)
                                 -Hrho*k1_*c/(k2_+c) * c, q2);
```

```
Expr adjoint1 = Integral(interior_, (lrho - lrho1_ )*lrhoHat/deltaT *deltaT

                                 +0.5*(D_/rhoB_)*((grad*lrhoHat)*(grad*c0_))*lrho*deltaT
                                 -0.5*k1_*dHlrho*c0_/(k2_+c0_)*lc*lrhoHat

                                 +0.5*(D_/rhoB_)*((grad*lrhoHat)*(grad*c1_))*lrho1_ *deltaT
                                 -0.5*k1_*dHlrho1*c1_/(k2_+c1_)*lc*lrhoHat

                                 +(lrho - lrho1_ )/deltaT
                                   *atau*(D_/rhoB_)*((grad*at2)*(grad*lrhoHat))
                                 +0.5*(D_/rhoB_)*((grad*lrho)*(grad*c0_))*lrho
                                   *atau*(D_/rhoB_)*((grad*at2)*(grad*lrhoHat))
                                 -0.5*k1*dHlrho*c0_/(k2_+c0_)*lc
                                   *atau*(D_/rhoB_)*((grad*at2)*(grad*lrhoHat))
                                 +0.5*(D_/rhoB_)*((grad*lrho1_)*(grad*c1_))
                                   *atau*(D_/rhoB_)*((grad*at2)*(grad*lrhoHat))
                                 -0.5*k1*dHlrho1_*c1_/(k2_+c1_)*lc
                                   *atau*(D_/rhoB_)*((grad*at2)*(grad*lrhoHat))

                                 -D_*(grad*lc)*(grad*lcHat)
                                 -Hlrho*k1_*k2_/((k2_+c0_)*(k2_+c0_))*lc*lcHat
                                 +(D_/rhoB_)*lrho*((grad*lcHat)*(grad*rho0_))*del,q2)  ;
Expr adjoint2 = adjoint1
          + Integral(interior_, 0.5*lrhoHat*(rho1_ - rhoTarget1_ )*boolExpr_*deltaT, q2)
          + Integral(interior_, 0.5*lrhoHat*(rho0_ - rhoTarget0_ )*boolExpr_*deltaT, q2) ;
```

Biofilm Inversion Formulation and implementation: Approach 2

The PDE constrained optimization problem

$$\min_{\rho,\rho_o} \mathcal{F}(\rho,\rho_u) = \frac{1}{2}\sum_{i=0}^{N}\int_0^T\int_\Omega(\rho-\rho^*)^2\delta(x-x_i)\,\mathbf{dx}\,\mathbf{dt} + \frac{\beta}{\mathbf{2}}\int_\Omega \rho_0^2\,\mathbf{dx}$$

subject to:

$$\begin{aligned}
\frac{\partial\rho}{\partial t} + \frac{D}{\rho_b}\nabla c\cdot\nabla\rho &= 0 && \text{in } \Omega\times[0,T]\\
\rho &= \rho_0 && \text{in } \Omega\times\{t=0\}.\\
D\Delta c &= \frac{k_1 c\rho}{k_2+c} && \text{in } \Omega\\
c &= c_D && \text{in } \Gamma_D
\end{aligned}$$

Additional complications:

- SUPG
- Crank-Nicholson

```
Expr state = Integral(interior_, (rho - rho0_)*rhoHat/deltaT
                              +0.5*(D_/rhoB_)*((grad*rho)*(grad*c))*rhoHat
                              +0.5*(D_/rhoB_)*((grad*rho0_)*(grad*c0_))*rhoHat

                              +(rho - rho0_)/deltaT
                                *stau*(D_/rhoB_)*((grad*st2)*(grad*rhoHat))
                              +0.5*(D_/rhoB_)*((grad*rho)*(grad*c))*rhoHat
                                *stau*(D_/rhoB_)*((grad*st2)*(grad*rhoHat))
                              +0.5*(D_/rhoB_)*((grad*rho0_)*(grad*c0_))*rhoHat
                                *stau*(D_/rhoB_)*((grad*st2)*(grad*rhoHat))

                              -D_*(grad*c)*(grad*cHat)
                              -Hrho*k1_*c/(k2_+c) * c, q2);
```

```
Expr lag = Integral(interior, 0.5*pow(u - target, 2.0)*direcDelta + R*alpha*alpha, q2)
  + Supg_CN_Integral;

Expr lagBC = EssentialBC(top, lambda*u=1.0, q2);

Functional L(mesh, lag, lagBC, vecType);

NonlinearOperator<double> stateProb = F.nonlinearVariationalProb(lambda, lambda0,
                                                                  rho, rho0,
                                                                  alpha, alpha0);

NOXSolver solver(noxParams, stateProb);
solver.solve() ;
```

Preliminary Inversion Results

(Realizations shown at final timestep)

The PDE constrained optimization problem

$$\min_{\rho,\rho_o} \mathcal{F}(\rho,\rho_u) = \frac{1}{2}\sum_{i=0}^{N}\int_0^T \int_\Omega (\rho-\rho^*)^2\delta(x-x_i)\,\mathbf{dx}\,\mathbf{dt} + \frac{\beta}{2}\int_\Omega \rho_0^2\,\mathbf{dx}$$

subject to:

$$\begin{aligned}
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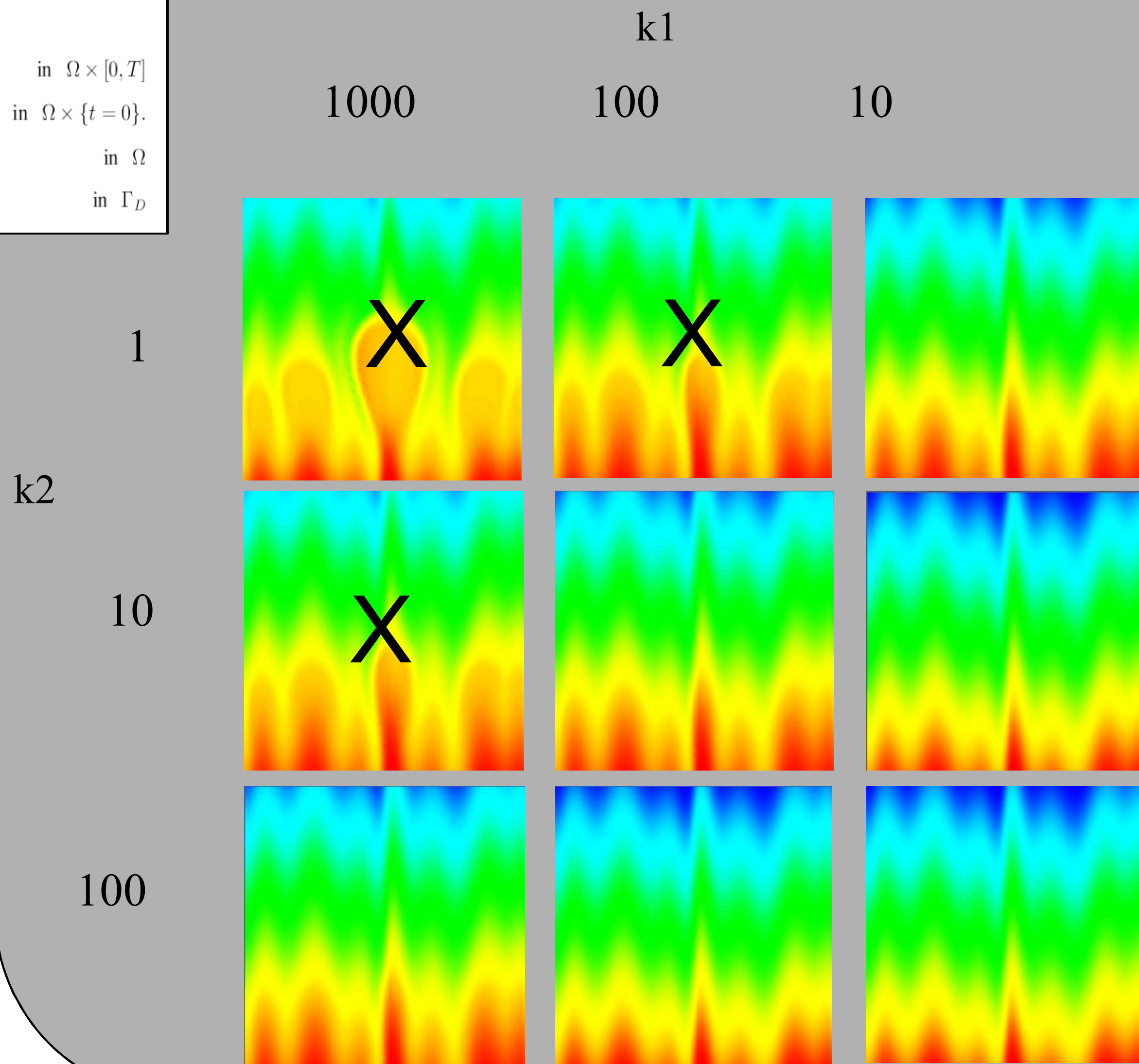
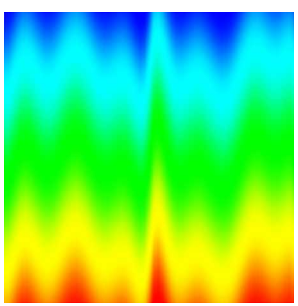
D\Delta c &= \frac{k_1 c\rho}{k_2+c} && \text{in } \Omega\\
c &= c_D && \text{in } \Gamma_D
\end{aligned}$$



<u>Inversion Details</u>:

- deltaT = 0.005
- grid 64x64
- R=0.0001
- QN-BFGS



Initial Condition

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Summary

- Work on biofilm is motivated by range of industrial applications
- Extensive physics defines biofilms dynamics: deposition, transport and detachment
- Inversion of IC or material parameters requires extensive formulation
- Efficient PDECO toolkit isolates users from implementation cost and errors
- Reconstruction of level set function needs to be investigated