Department Review FY06

Large Scale Intrusive Optimization and Applications

Bart van Bloemen Waanders

Optimization and Uncertainty Estimation (1411)

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FY06 Overview

Research

- Decontamination LDRD (Frink, Altman, Bader, Hill)
- Completing poroelasticity inversion (Hetmaniuk)
- Scalable interface (Thyra::ModelEvaluator) for next generation supercomputers (Red Storm) SC06 (Bartlett & Long)
- Lab and simulation network LDRD, EPA water security project completion, ROM, MG velocity inversion, uncertainty quantification through large scale inversion
- Publications (2 journal, 1 SC06, 1 book, 4 conference papers, 2 book chapters, 1 rather large SAND report)

Programmatic

- SciDAC proposal SciOps Institute for Optimization (Ghattas)
- DTRA proposal
- LDRD, CSRF proposals

Outreach

- Taught numerical optimization class (UNM)
- Publishing 2nd PDE constrained optimization book (SIAM book series on Computational Science and Engineering)
- New collaboration with M. Wheeler (UT): real time reservoir modeling

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Publications FY06

1. A **Scalable Optimization Interface** for Numerical Simulation Applied to the Next Generation Supercomputer, R. Bartlett, K. Long, B. van Bloemen Waanders, SC06
2. Inversion of Airborne Contaminants in a Regional Model, Volkan Akcelik, George Biros, Andrei Draganescu, Omar Ghattas, Judith Hill, and Bart van Bloemen Waanders, **Lecture Notes in Computer Science,** Springer Verlag, Editors: Vassil N. Alexandrov, Geert Dick van Albada, Peter M.A. Sloot, Jack Dongarra 2006
3. V. Akcelik, G. Biros, O. Ghattas, J. Hill, D. Keyes, and B. van Bloemen Waanders, "Parallel algorithms for PDE-constrained optimization", in **Frontiers of Parallel Computing**, M. Heroux, P. Raghaven, H. Simon, eds, SIAM, 2006
4. Algorithm and Simulation Development in Support of **Response Strategies for Contamination** Events in Air and Water Systems, B. van Bloemen Waanders (Editor), SAND Report SAND2006-0074, January 2006
5. Goal-Oriented, Model Constrained Optimization for **Reduction of Large Scale Systems** T. Bui-Thanh, K. Willcox, O. Ghattas, B. van Bloemen Waanders, Journal Computational Physics, 2006
6. **Hybrid Differentiation** Strategies for Simulation and Analysis of C++ codes, R. Bartlett, B. van Bloemen Waanders, M. Berggren, ACM TOMS, 2006
7. Real Time PDE Constrained Optimization, L. Biegler, O. Ghattas, M. Heinkenschloss, D. Keyes, B. van Bloemen Waanders (Editors) **SIAM Book Series** on Computational Science and Engineering 2006

(In Preparation due June 1, 2006)

1. *Numerical Simulation and Experimental Validation of **Biofilms** during Contamination Events, B. van Bloemen Waanders, L. Frink, B. Bader,. J. Hill, S. Altman, WDSA conference Cincinnati 2006*
2. *Source Inversion Using Changes in Water Quality Parameter, J. Hill, B. van Bloemen Waanders, C. Laird WDSA conference Cincinnati 2006*
3. *Real Time Water Demand Estimation in Water Distribution System through Extended **Kalman Filtering** F. Sheng, J. Uber, D. Bocceli. B. van Bloemen Waanders, R. Janke, WDSA Conference. Cincinnati 2006*
4. *High Fidelity Computational Fluid Dynamics for Water Distribution Systems, S. Webb, B. van Bloemen Waanders, WDSA conference Cincinnati 2006*

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Decontamination LDRD Project: General Description

- **General description**: Support the decontamination process in water distribution systems

- **More specifically**: Evaluate the role of biofilms

- **Strategy**: develop multi-physics simulation capabilities to predict the structure, thermodynamics, and flow related properties of biofilms; use optimization (under uncertainty) for model calibration and control strategies

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Decontamination LDRD Project: Biofilms

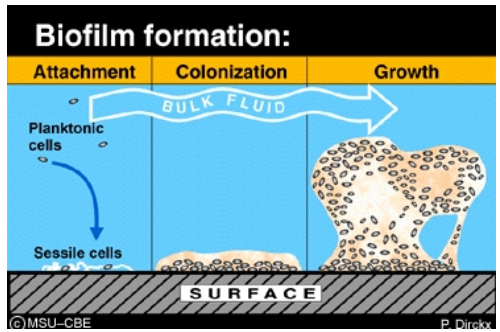
Description:

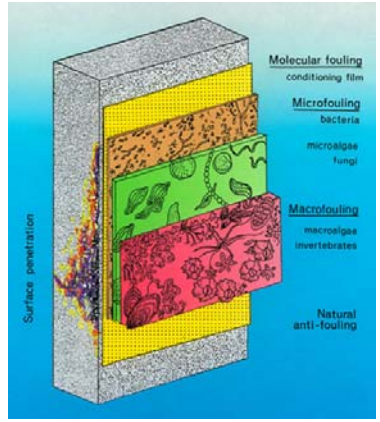
• Biofilm forms when bacteria adhere to surfaces in aqueous environments and begin to excrete a slimy, glue-like substance that can anchor them to all kinds of material (such as metals, plastics, soil particles, medical implant materials, and tissue.)

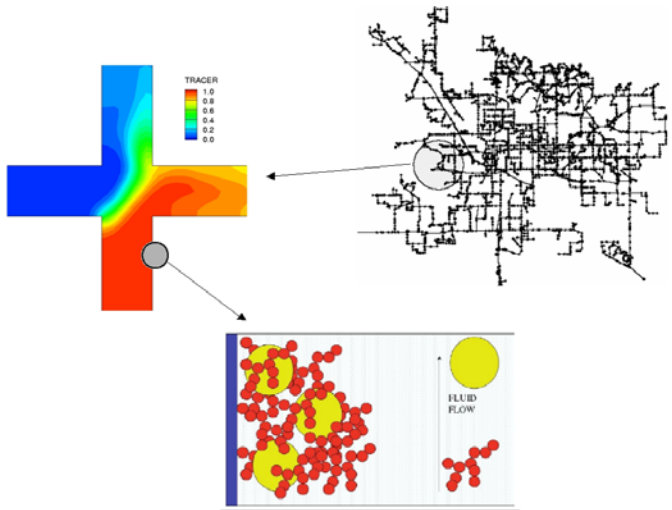
• Biofilms consist of many species of bacteria, as well as fungi, algae, protozoa, debris and corrosion products.

Impact: water distribution systems, dental, food, biofouling, sewage industry, human physiology

Technical challenges: multi-physics, multi-scale, micro-hydrodynamics, requiring accurate description of structure, thermodynamics properties, chemistry, optimization and uncertainty quantification.







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Decontamination LDRD Project: Progress

- **Molecular modeling** – develop biofilm model using DFT approach; goal is to characterize structure/thermodynamic properties and couple to hydrodynamics
- **Diffusion model** – two diffusion region to address change at interface
- **Convection-diffusion-reaction** - 3D finite element prediction capability, with rSQP based optimization algorithms for control and parameter estimation.
- **Navier Stokes** - coupling at molecular level, develop appropriate diffusion and viscosity models
- **Validation** – experimental, model calibration
- **Enabling technologies** – SQP Optimization, multi-period, ROM

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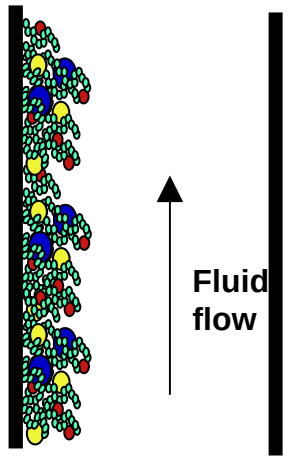
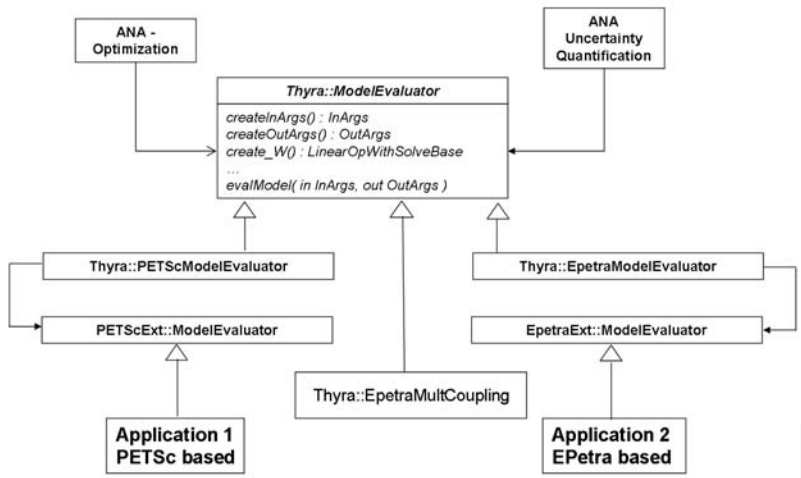
Decontamination LDRD Project: Progress Molecular Modeling

Tramonto: prototype biofilm model with semi permeable EPS, 2 macromolecules, and 1 chemical species

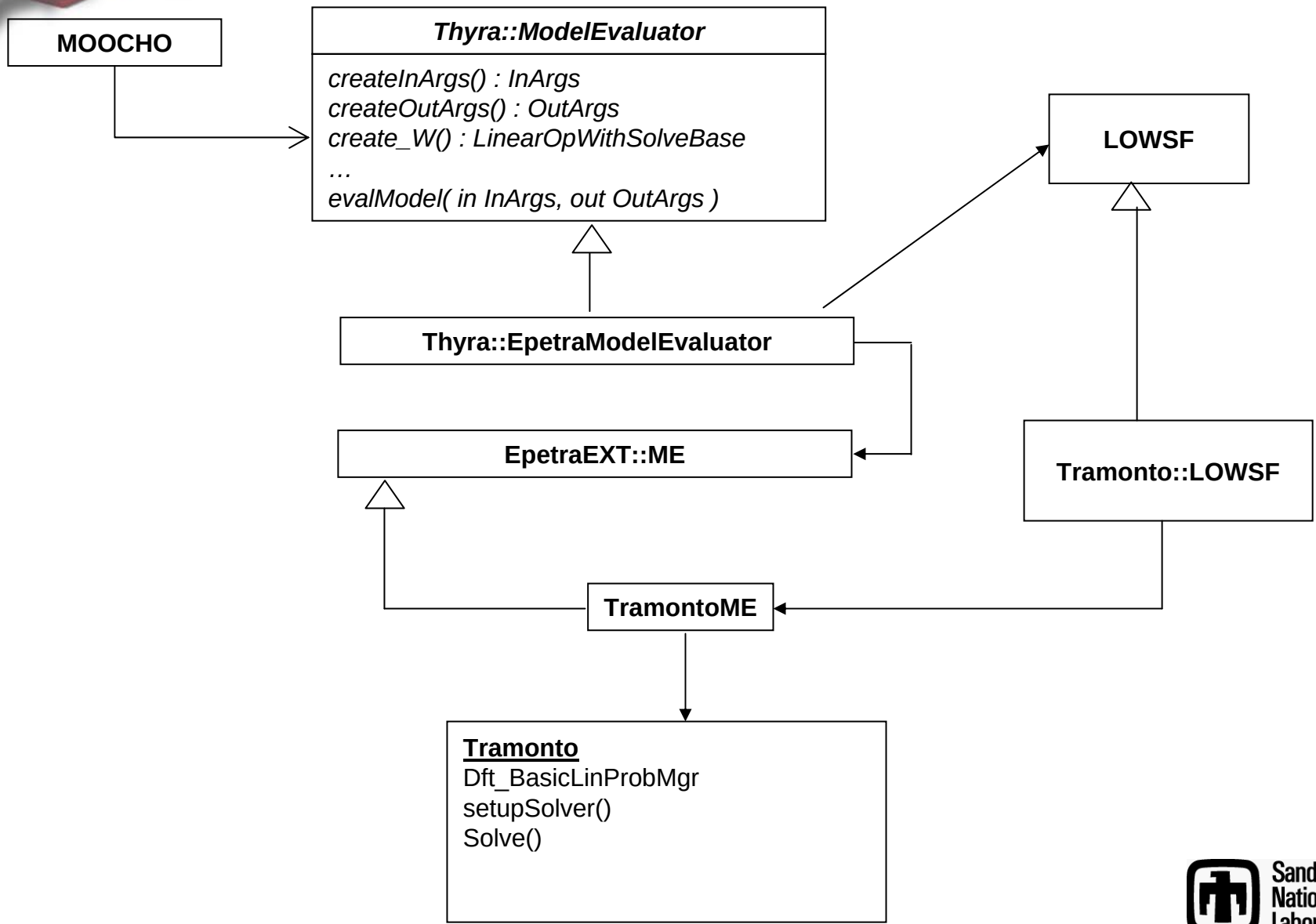


Optimization: interface through the Thyra::ModelEvaluator



Application: control of decontamination at biofilm scale, and parameter estimation

Decontamination LDRD Project: Tramonto ModelEvaluator



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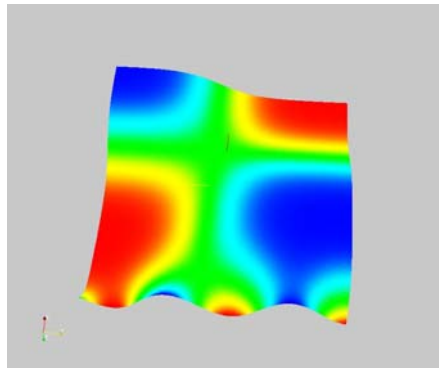
Decontamination LDRD Project: Progress Macro Modeling

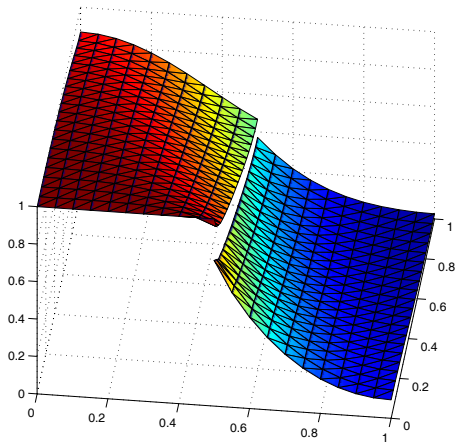
- Macro-model: 3D finite element based CDR Control

$$
\begin{aligned}
\min_{y,u} \quad & \frac{1}{2}\int_{\Omega}(y-y^*)^2 dx + \frac{1}{2}\int_{\partial\Omega} u^2 dx \\
\text{s.t.} \quad & (v\cdot\nabla)y = D\nabla^2 y + y(\alpha+\beta y^2) \\
& \frac{\partial y}{\partial n} = u
\end{aligned}
$$



- Two region diffusion model

$$
\begin{aligned}
\frac{\partial y}{\partial t} + (v\cdot\nabla)y &= D\nabla^2 y - k_r y \\
\frac{\partial y}{\partial n} &= M(y_w - \tfrac{y_b}{H})
\end{aligned}
$$



Decontamination LDRD Project: Next Steps

- Demonstrate optimization capability in Tramonto for parameter estimation and control
- Develop multi-physics consisting of CDR-molecular modeling
- Develop micro-hydrodynamics version of Navier Stokes
- Apply algorithmic capabilities to other applications

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Summary and Future Work

FY 2006 activities:

- Decontamination LDRD
- Poroelasticity inversion
- Scalable interface for next generation supercomputers
- Numerical optimization class
- SciDAC proposal Institute for Optimization (SciOps)
- Real time reservoir modeling
- Publications (11)

Additional future activities:

- Fall UNM class : Nonlinear unconstrained optimization
- Velocity inversion with MG preconditioning
- Goal oriented reduced order modeling
- Uncertainty estimation through large scale optimization methods
- Next generation design based simulation for micro/nano flows.

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