Numerical Simulation and Optimization in Natural Sciences and Engineering

contributions, present work, and perspectives

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Simulation and optimization

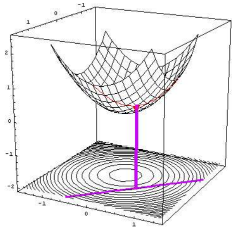
Aim of numerical simulation is to achieve better understanding of real world systems

eventually with the purpose of influencing or modifying these systems

thus motivating the formulation of optimization problems

multigrid strategies appear to be the method of choice for large-scale simulation and optimization

Constrained optimization problems



$$\begin{cases} \text{minimize} & J(y,u,y_d) \\ \text{under the constraint} & e(y,u)=0 \end{cases}$$

- A model of the dynamical or equilibrium system
- A description of the optimization mechanism
- A criterion that models the purpose of optimization

Optimality systems

Consider the constrained minimization problem

$$\begin{array}{ll} \min_{u \in U_{ad}} J(y,u) & J : Y \times U \to \mathbb{R} \\ \text{s.t.} \quad e(y,u) = 0 & \text{where } e_y^{-1} \text{ exists.} \end{array}$$

The existence of e_y^{-1} enables a clear distinction between y, the state variable, and $u \in U_{ad}$, the optimization variable in the admissible set. Assume an objective functional given by

$$J(y,u) = h(y) + \nu g(u), \qquad \nu \geq 0$$

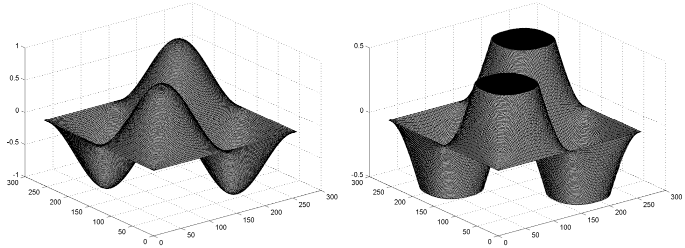
The solution of this optimization problem is characterized by the following optimality system

$$\begin{aligned} e(y,u) &= 0 \\ e_y(y,u)^* p &= -h'(y) \\ (\nu g'(u) + e_u^* p, v - u) &\geq 0 \text{ for all } v \in U_{ad} \end{aligned}$$

Control-constrained optimization

$$\begin{aligned} \Delta y + y^4 &= u + f, \\ \Delta p + 4y^3 p &= -(y - z) \\ (\nu u - p, v - u) &\geq 0 \quad \text{for all } v \in U_{ad} \end{aligned}$$

$$U_{ad} = \{u \in L^2(\Omega) \mid -1/2 \leq u(\mathbf{x}) \leq 1/2 \text{ a.e. in } \Omega\}$$



Multigrid solution for $\nu = 10^{-6}$. The state (left) and the control (right). $z(x_1, x_2) = \sin(2\pi x_1)\sin(2\pi x_2) + O(\nu)$

Simulation and optimization of evolutionary systems

Simulation and control can be required to investigate evolution, track a desired trajectory $y_d(\mathbf{x},t)$ or reach a desired terminal state $y_T(\mathbf{x})$.
For these purposes, the following cost functional is considered

$$J(y,u) = \frac{\alpha}{2}||y - y_d||^2_{L^2(Q)} + \frac{\beta}{2}||y(\cdot,T) - y_T||^2_{L^2(\Omega)} + \frac{\nu}{2}||u||^2_{L^2(Q)}$$

For reaction-diffusion models, the optimality system is given by

$$\begin{aligned} -\partial_t y + G(y) + \sigma\Delta y &= u \quad \text{in } Q \\ \partial_t p + G'(y)p + \sigma\Delta p + \alpha(y - y_d) &= 0 \quad \text{in } Q \\ \nu u - p &= 0 \quad \text{in } Q \end{aligned}$$

With initial condition $y(\mathbf{x},0) = y_0(\mathbf{x})$ for the state variable (evolving forward in time). And terminal condition for the adjoint variable (evolving backward in time) $p(\mathbf{x},T) = \beta(y(\mathbf{x},T) - y_T(\mathbf{x}))$.

Multigrid methods for PDE simulation and optimization

Multigrid FAS framework to solve $A_h(w_h) = f_h$

Set $B_1(w_1^{(0)}) \approx A_1^{-1}$. For $k = 2, \ldots, L$ define B_k in terms of B_{k-1} as follows.

1. Set the starting approximation $w_k^{(0)}$.
2. Pre-smoothing. Define $w_k^{(l)}$ for $l = 1, \ldots, m_1$, by
$$w_k^{(l)} = S_k(w_k^{(l-1)}, f_k).$$
3. Coarse grid correction.
Set $w_k^{(m_1+1)} = w_k^{(m_1)} + I_{k-1}^{k}(w_{k-1} - \hat{I}_k^{k-1} w_k^{(m_1)})$ where
$$w_{k-1} = B_{k-1}(\hat{I}_k^{k-1} w_k^{(m_1)}) \left[I_k^{k-1}(f_k - A_k(w_k^{(m_1)})) + A_{k-1}(\hat{I}_k^{k-1} w_k^{(m_1)}) \right].$$
4. Post-smoothing. Define $w_k^{(l)}$ for $l = m_1 + 2, \cdots, m_1 + m_2 + 1$, by
$$w_k^{(l)} = S_k(w_k^{(l-1)}, f_k).$$
5. Set $B_k(w_k^{(0)}) f_k = w_k^{(m_1+m_2+1)}$.

Collective smoothing

Obtain y_{ij} and p_{ij} as functions of u_{ij} as follows

$$
\begin{array}{rcl}
-\Delta_h y_h - u_h & = & f_h \rightarrow \quad y_{ij}(u_{ij}) \; = \; (A_{ij} - h^2 u_{ij})/c^y_{ij}, \\
-\Delta_h p_h + y_h & = & z_h \rightarrow \quad p_{ij}(u_{ij}) \; = \; (c^y_{ij} B_{ij} + h^2 A_{ij} - h^4 u_{ij})/(c^p_{ij} c^y_{ij}) \\
(\nu u_h - p_h)\cdot(v_h - u_h) & \geq & 0
\end{array}
$$

The solution of the unconstrained problem satisfies

$$J'(y(\tilde{u}),\tilde{u}) = \nu \tilde{u}_{ij} - p_{ij}(\tilde{u}_{ij}) = 0.$$

The update value for u_{ij} is obtained by projection

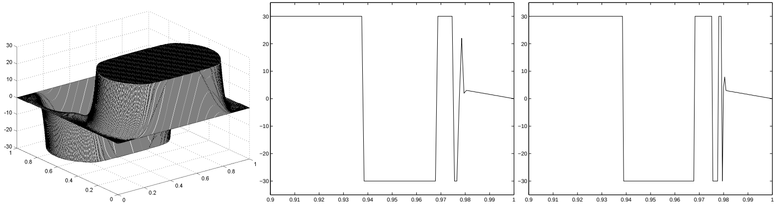
$$
u_{ij} = \begin{cases} u_{H\,ij} & \text{if } \tilde{u}_{ij} > u_{H\,ij} \\ \tilde{u}_{ij} & \text{if } u_{L\,ij} \leq \tilde{u}_{ij} \leq u_{H\,ij} \\ u_{L\,ij} & \text{if } \tilde{u}_{ij} < u_{L\,ij} \end{cases}
$$

For $U_{ad} = L^2(\Omega)$, smoothing factor $\mu \approx 0.5$ almost independent of ν and h.

Bang-bang and chattering phenomena

Consider the objective function $z(x_1, x_2) = \sin(2\pi x_1)\sin(\pi x_2)$ and box constraints $u_L = -30$ and $u_H = 30$.

Results for $\nu = 10^{-6}$ and $\nu = 0$.



Bang-bang and switching of the control function for $x_1 = 3/4$ and $x_2 \in [0.9, 1]$ obtained with $\nu = 0$ on increasingly finer meshes: 1025×1025 and 8193×8193.

Multigrid convergence theory

1. Multigrid convergence theory for scalar elliptic equation

$$-\Delta y = f \text{ in } \Omega \text{ and } y = 0 \text{ on } \partial\Omega.$$

The matrix form of this problem is $\hat{A}_k y_k = f_k$.

Convergence results are given in terms of the error operator $\hat{E}_k := I_k - \hat{B}_k \hat{A}_k$. We have (for $m_1 = 1$, $m_2 = 0$)

$$\hat{E}_k y = [(I_k - I^k_{k-1}\hat{P}_{k-1}) + I^k_{k-1}\hat{E}_{k-1}\hat{P}_{k-1}]\hat{S}_k y.$$

Theorem 1: There exists a positive constant $\hat{\delta} < 1$ such that

$$(\hat{A}_k \hat{E}_k y, \hat{E}_k y)_k \le \hat{\delta}^2 (\hat{A}_k y, y)_k \quad \text{for all } y \in M_k,, \qquad k = L$$

2. Consider the decoupled symmetric system

$$\begin{aligned} -\nu\Delta y &= \nu g && \text{in } \Omega, \\ y &= 0 && \text{on } \partial\Omega, \\ -\Delta p &= z && \text{in } \Omega, \\ p &= 0 && \text{on } \partial\Omega. \end{aligned}$$

This system is exactly two copies of Poisson problem. Hence the multigrid convergence theory for this system inherits the properties of the scalar case.

3. To analyze the optimality system define

$$\hat{\mathscr{A}}_k = \begin{pmatrix} \nu\hat{A}_k & 0 \\ 0 & \hat{A}_k \end{pmatrix}$$

and analogously $\hat{\mathscr{B}}_k$, $\hat{\mathscr{E}}_k$, etc., as counterparts of $\hat{B}_k$, $\hat{E}_k$, etc..

Theorem 2: There exists a positive constant $\hat{\delta} < 1$ such that

$$(\hat{\mathscr{A}}_L \hat{\mathscr{E}}_L \mathbf{w}, \hat{\mathscr{E}}_L \mathbf{w})_L \le \hat{\delta}^2 (\hat{\mathscr{A}}_L \mathbf{w}, \mathbf{w})_L \quad \text{for all } \mathbf{w} = (y,p) \in \mathscr{M}_L,$$

Consider

$$\mathscr{A}_k = \hat{\mathscr{A}}_k + \mathscr{D}_k,$$

where

$$\mathscr{D}_k = \begin{pmatrix} 0 & -I_k \\ I_k & 0 \end{pmatrix}.$$

Note that $|(\mathscr{D}_k(u,v),(y,p))| \le C\,|(u,v)|\,|(y,p)|$.

With $\mathscr{B}_k$, $\mathscr{A}_k$, etc., replacing $\hat{B}_k$, $\hat{A}_k$, etc..

$$\mathscr{E}_k = [\mathscr{I}_k - \mathscr{I}^k_{k-1}\mathscr{P}_{k-1} + \mathscr{I}^k_{k-1}\mathscr{E}_{k-1}\mathscr{P}_{k-1}]\mathscr{S}_k$$

Theorem 3: There exist positive constants h_0 and $\delta < 1$ such that for all $h_1 < h_0$ we have

$$(\hat{\mathscr{A}}_k \mathscr{E}_k \mathbf{w}, \mathscr{E}_k \mathbf{w})_k \le \delta^2 (\hat{\mathscr{A}}_k \mathbf{w}, \mathbf{w})_k \quad \text{for all } \mathbf{w} \in \mathscr{M}_k, \qquad k = L$$

Space-time multigrid convergence estimates

Realize the coupling between state and control variables. Preserve the opposite time orientation of state and adjoint equations.
Reaction-diffusion models optimality system

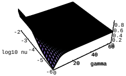
$$
\begin{array}{rcll}
-\partial_t y + G(y) + \sigma \Delta y & = & u & \text{in } Q \\
\partial_t p + G'(y) p + \sigma \Delta p + \alpha (y - y_d) & = & 0 & \text{in } Q \\
\nu u - p & = & 0 & \text{in } Q
\end{array}
$$

Discretization by backward Euler scheme.

Time-Splitted Collective Gauss-Seidel Iteration (TS-CGS)

1. Set the starting approximation.
2. For $m = 2, \ldots, N_t$ do
3. For *ij* in, e.g., lexicographic order do

$$
\begin{array}{rcl}
y^{(1)}_{ijm} & = & y^{(0)}_{ijm} + F_y[r_y(w), r_p(w)] \\
p^{(1)}_{ijN_t-m+2} & = & p^{(0)}_{ijN_t-m+2} + F_p[r_y(w), r_p(w)]
\end{array}
$$



Smoothing factor of TS-CGS scheme as function of ν and γ

Time-Line Collective Gauss-Seidel Iteration (TL-CGS)

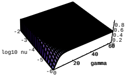
1. Set the starting approximation.
2. For *ij* in, e.g., lexicographic order do

$$
\begin{pmatrix} y \\ p \end{pmatrix}^{(1)}_{ij} = \begin{pmatrix} y \\ p \end{pmatrix}^{(0)}_{ij} + M^{-1} \begin{pmatrix} r_y \\ r_p \end{pmatrix}_{ij}
$$

The block-tridiagonal system has the following form

$$
M = \begin{bmatrix}
A_2 & C_2 & & \\
B_3 & A_3 & C_3 & \\
 & & C_{N_t} & \\
 & B_{N_t+1} & A_{N_t+1} &
\end{bmatrix}
$$

Centered at t_m, the entries B_m, A_m, C_m refer to the variables (y, p) at t_{m-1}, t_m, and t_{m+1}, respectively.
Block-tridiagonal systems can be solved with $\mathcal{O}(N_t)$ effort.



Smoothing factor of TL-CGS scheme as function of ν and $\gamma = \delta t / h^2$

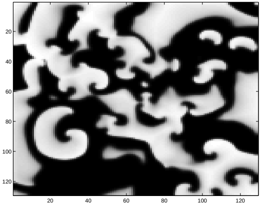
Simulation and optimization problems

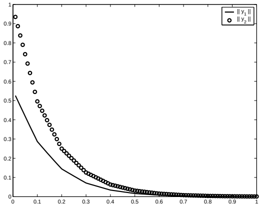
Cardiac arrhythmia and defibrillation

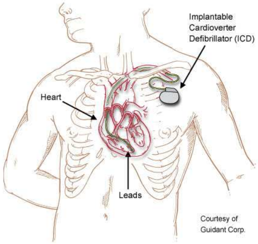
Consider the Aliev-Panfilov model of cardiac cell tissue dynamics

$$
\begin{aligned}
\frac{\partial y_1}{\partial t} &= -k y_1 (y_1 - a)(y_1 - 1) - y_1 y_2 + \sigma \Delta y_1 + u \\
\frac{\partial y_2}{\partial t} &= [\varepsilon_0 + \frac{\mu_1 y_2}{\mu_2 + y_1}][-y_2 - k y_1 (y_1 - b - 1)]
\end{aligned}
$$

y_1: transmembrane potential; y_2: the membrane conductance.







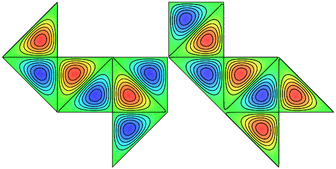
Electrical field control response driving the system from a turbulent electrical pattern to a uniform pattern as in the case of no stimulus.

Eigenvalue computation $A\phi^i = \lambda^i B\phi^i$

FAS-AMG($A_k, B_k, F_k, \phi_k^i, \lambda_k^i$)
begin
 if k is the coarsest level then
  apply $\mathscr{S}_k$, m_c times, on $A_k\phi_k^i - \lambda_k^i B_k \phi_k^i = F_k$
 else
  apply $\mathscr{S}_k$, m_1 times, on $A_k\phi_k^i - \lambda_k^i B_k \phi_k^i = F_k$
  $\phi_{k+1}^i = I_k^{k+1}\phi_k^i$
  $F_{k+1} = (A_{k+1} - \lambda_k^i B_{k+1})\phi_{k+1}^i + I_k^{k+1}[F_k - (A_k - \lambda_k^i B_k)\phi_k^i]$
  call FAMG($A_{k+1}, B_{k+1}, F_{k+1}, \phi_{k+1}^i, \lambda_k^i$)
  $\phi_k^i = \phi_k^i + I_{k+1}^k\left(\phi_{k+1}^i - I_k^{k+1}\phi_k^i\right)$
  apply $\mathscr{S}_k$, m_2 times, on $A_k\phi_k^i - \lambda_k^i B_k \phi_k^i = F_k$
 endif

FAMG($A_h, B_h, [\phi_h^1, \ldots, \phi_h^{ne}], [\lambda_h^1, \ldots, \lambda_h^{ne}]$)
Compute $\left(\lambda_L^i, \phi_L^i\right)$, $i = 1, \ldots, n_e$, (QR algorithm).
for $k = L-1, \ldots, 1$ do
 for $i = 1, \ldots, n_e$ do
  $\phi_k^i = I_{k+1}^k \phi_{k+1}^i$
  call FAS-AMG ($A_k, B_k, 0, \phi_k^i, \lambda_k^i$)
 done
 call Ritz$\left(A_k, B_k, \left[\phi_k^1, \ldots, \phi_k^{ne}\right], \left[\lambda_k^1, \ldots, \lambda_k^{ne}\right]\right)$

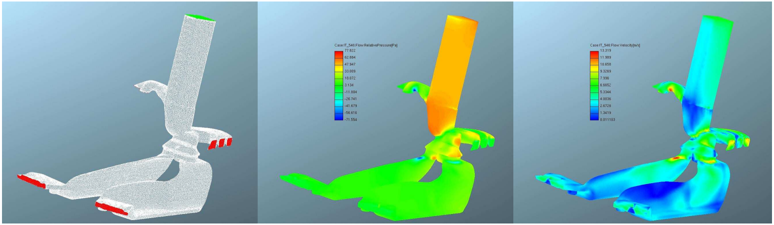
	FAMG	PAMG	LAMG
λ_e	λ_h	λ_h	λ_h
29.59867	29.67345	29.67345	29.67345
59.15680	59.47530	59.47530	59.47530
59.15680	59.47539	59.47539	59.47539
59.15680	59.47624	59.47624	59.47624
88.71493	89.40694	89.40694	89.40694
88.71493	89.40747	89.40747	89.40747
88.71493	89.40925	89.40925	89.40925
108.5656	109.4311	109.4311	109.4311
108.5656	109.4330	109.4330	109.4330
108.5656	109.4349	109.4349	109.4349



Isospectral drums with the 9th mode.

Industrial numerical simulations

AMG Calculations for a ventilation duct ($k - \varepsilon$, $Re \approx 10^5$).
Mesh 564616 cells
417826 tetrahedral cells and 146790 prismatic cells (wall layer).
CPU Time AMG: 8496 / PCG: 12308



VW Benchmark - Ventilation duct: geometry, relative pressure, velocity. Project SWIFT/FIRE AMG. Courtesy of AVL List GmbH.

Optical flow

Optimal control formulation of the optical flow problem: Find $\vec{w} = (u,v)$ s.t.

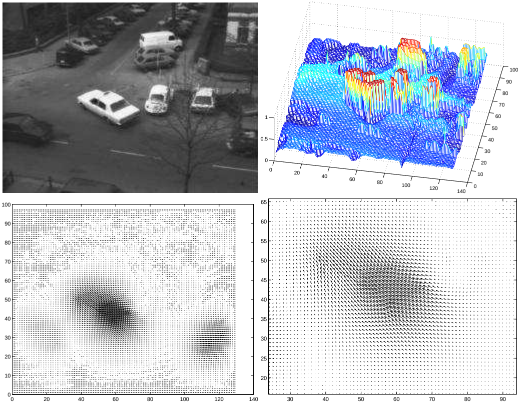
$$\min_{\vec{w}\in C} J(I(\vec{w}),\vec{w}),$$

$$I_t + \vec{w}\cdot\nabla I = 0, \quad I(\cdot,0) = Y_1,$$

J is a cost functional of the tracking type with respect to a sampled sequence of image frames $\{Y_k\}_{k=1}^N$, at times t_k.
Solve the following elliptic-hyperbolic optimality system

$$\begin{aligned}
I_t + \vec{w}\cdot\nabla I &= 0\\
I(\cdot,0) &= Y_1\\
p_t + \nabla\cdot(\vec{w}p) &= \sum_{k=2}^{N-1}[\delta(t-t_k)(I(\cdot,t_k)-Y_k)]\\
p(\cdot,T) &= -(I(\cdot,T)-Y_N)\\
\alpha\frac{\partial^2 u}{\partial t^2} + \beta\Delta u + \gamma\frac{\partial}{\partial x}(\nabla\cdot\vec{w}) &= p\frac{\partial I}{\partial x}\\
\alpha\frac{\partial^2 v}{\partial t^2} + \beta\Delta v + \gamma\frac{\partial}{\partial y}(\nabla\cdot\vec{w}) &= p\frac{\partial I}{\partial y}
\end{aligned}$$

Optical flow from a sequence of images



First frame of the Taxi Sequence (top left); the corresponding brightness distribution (top right). Optical flow for the Taxi Sequence (bottom left).

Close-ups of the solution containing the region of the taxi (bottom right).

Bose Einstein condensates in magnetic microtraps

The dynamics of the condensate is described by the Gross-Pitaevskii equation

$$i\dot{\psi}(r,t) = \left(-\frac{1}{2}\nabla^2 + V(r,\lambda(t)) + g\,|\psi(r,t)|^2\right)\psi(r,t),$$

where $V(r,\lambda(t))$ is a control potential depending on $\lambda(t)$. We require to minimize

$$J(\psi,\lambda) = \frac{1}{2}\left(1 - \left|\langle\psi_d|\psi(T)\rangle\right|^2\right) + \frac{\gamma}{2}\int_0^T \left(\dot{\lambda}(t)\right)^2 dt$$

Consider the varying single-to-double-well potential

$$V(x,\lambda) = \begin{cases} \frac{1}{2}\left(|x| - \frac{\lambda d}{2}\right)^2 & \text{for } |x| > \frac{d}{4} \\ \frac{1}{2}\left(\frac{(\lambda d)^2}{8} - x^2\right) & \text{otherwise,} \end{cases}$$

single-well potential for $\lambda = 0$; double-well potential for $\lambda = 1$.

Optimality system: Coupled NLSE

The optimal solution is obtained solving

$$i\dot{\psi} = \left(-\frac{1}{2}\nabla^2 + V_\lambda + g|\psi|^2\right)\psi$$

$$i\dot{p} = \left(-\frac{1}{2}\nabla^2 + V_\lambda + 2g|\psi|^2\right)p + g\,\psi^2\,p^*$$

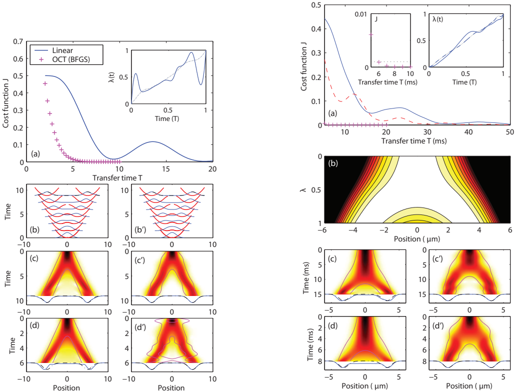
$$\gamma\ddot{\lambda} = -\Re e\langle\psi|\frac{\partial V_\lambda}{\partial\lambda}|p\rangle\,,$$

with the initial and terminal conditions

$$\begin{aligned} \psi(0) &= \psi_0 \\ i\,p(T) &= -\langle\psi_d|\psi(T)\rangle\,\psi_d \\ \lambda(0) &= 0\,, \quad \lambda(T) = 1\,. \end{aligned}$$

Splitting of Bose-Einstein condensate

Wavefunction splitting for linear t/T, square-root $\sqrt{t/T}$ (Hänsel *et al.*), and optimized variation of $\lambda(t)$.



(a) Cost function for linear t/T (solid line), square-root $\sqrt{t/T}$ (dashed line), and optimized (symbols) variation of $\lambda(t)$. The optimized $J(\psi,\lambda)$ is magnified in the left inset. The right inset reports the optimal $\lambda(t)$ for $T=8$ ms (solid line) and $T=15$ ms (dashed line). (b) Contour plot of magnetic confinement potential as a function of λ. (c,d) Wave function evolution for linear variation of λ and transfer times of (c) $T=15$ ms and (d) $T=8$ ms. (c',d') Same as (c,d) but for optimized control.

Perspectives

- High-performance computing in optimization.
- Multilevel optimization schemes.
- Time-dependent inverse problems.

Teaching, networking, meeting

- Teaching undergraduate and graduate students (1 PhD, 2 MSc).

  Analysis, Linear Algebra, Optimization, Complex Analysis, Ordinary Differential Equations, Programming in C++, Numerical Analysis, Theory of Partial Differential Equations, Multilevel methods in optimization with PDE models, Numerical Solution of Partial Differential Equations.

- Networking with excellent scientists.

  A.M. Anile (Catania), B. Basara (Graz), G. Biros (Penn), C.C. Douglas (Kentucky), O. Ghattas (Austin), M. Falcone (Roma), R. Griesse (RICAM), K. Ito (NCSU), K. Kunisch (Graz), Do.Y. Kwak (KAIST), A. Majorana (Catania), C. Meyer (Berlin), A. Rösch (RICAM), G. Russo (Catania), O. Scherzer (Innsbruck), J. Salomon (Paris VI), V. Schulz (Trier), E. Süli (Oxford), M. Vanmaele (Ghent), I. Yavneh (Technion),....

- Organizing meetings.

  Workshop Advances in Numerical Algorithms, Graz, 2003; GAMM 2006 Minisymposium "Multigrid Methods for Optimal Control of PDEs", Berlin; Conference "Domain Decomposition Methods DD17", St. Wolfgang/Strobl, 2006; SIAM Annual Meeting 2006 Minisymposium "Multilevel Methods for Optimization and Inverse Problems", USA, Boston, 2006; "ENUMATH 2007" Conference, Graz, 2007.

Academic and industrial projects

- Quantum optimal control of semiconductor nanostructures (FWF project P18136-N13)

- A computational framework for real-time identification of hazardous events (Biros, Willcox, et al.; NSF)
- Real time optimization for data assimilation and control of large scale dynamic simulations (Ghattas, Biros, et al.; NSF)
- Fast solvers for computational problems arising in pharmacy, life sciences, mathematics, physics, and the environment (Douglas, Langer et al.; NSF)

- SWIFT/FIRE AMG; PARALLEL SWIFT AMG; Boundary Conditions Calculation in BOOST; Perforated Pipes in BOOST; Multigrid Solution of the Reynolds Equation in EXCITE (WWW.AVL.COM)

Scientific contributions

- Algebraic and geometric multigrid methods for elliptic and parabolic PDEs and for optimality systems.
- Convergence theory of multigrid schemes for optimality systems.
- Numerical analysis of discretization schemes for linear and nonlinear elliptic and parabolic partial differential equations (PDE) and optimality systems.
- Algebraic multigrid methods for eigenvalue problems.
- Modeling and numerical solution of image problems.
- Modeling and numerical simulation of gas dynamics and hydraulic systems.
- Modeling, numerical simulation and control of quantum systems.

→ modeling → numerical approx. → simulation → numerical analysis → simulation → optimization → engineering

Outline