Multiscale Methods for Transient Simulation and Optimization

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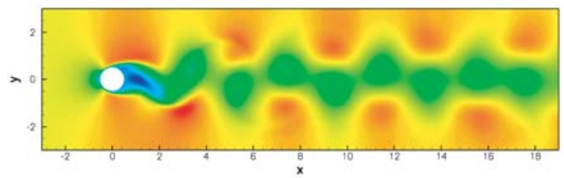
Research Roadmap



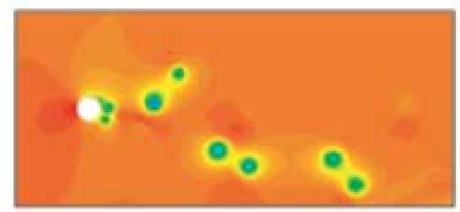
Transient Optimization

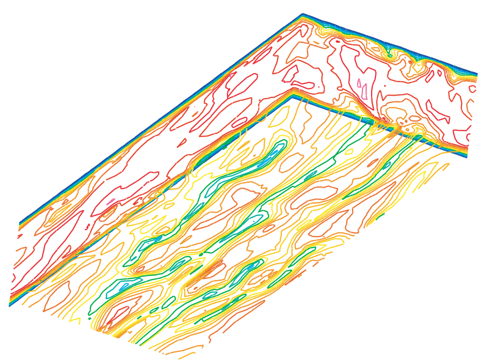
Active Flow Control

Discontinuous Galerkin

Turbulence Simulation (LES/DES)

Multiscale and Multifidelity Methods





Discontinuous Galerkin is an *enabling* algorithmic technology…

Contributions and Collaborations

Contributions

- *ASC Spatial Discretization*
  - Discontinuous Galerkin (DG)
  - Multiscale algorithms
  - Re-entry vehicles …
- *ASC Optimization*
  - DG + Optimization (DG-OPT)
  - Multiscale & multifidelity for optimization
  - Spin-up …
- *LDRD Homeland Security*
  - DG-OPT
  - Transient optimal control
  - Bio/Chem remediation …

Collaborations

9211 Ross Bartlett, Mike Eldred, Bart van Bloemen Waanders

9214 Pavel Bochev, Rich Lehoucq

9231 Mark Christon

9233 John Shadid

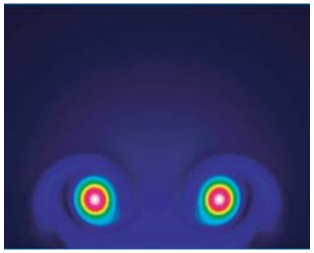
9235 Alex Slepoy

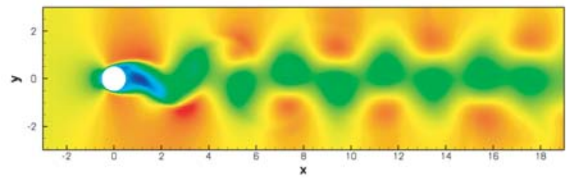
9115 Matt Barone, David Kuntz

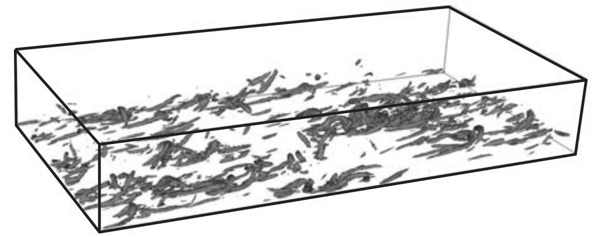
8752 Greg Wagner

Rice Gouquan Chen (PhD student), Matthias Heinkenschloss, Srinivas Ramakrishnan (PhD student)

Transient PDE Constrained Optimization

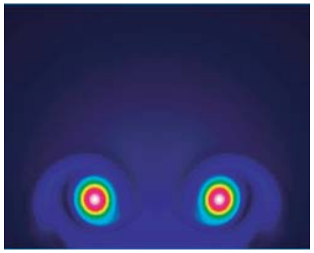


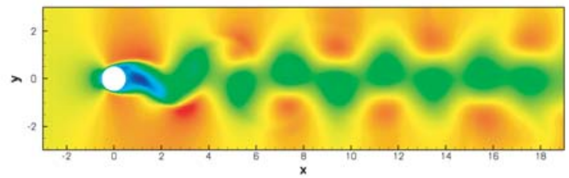


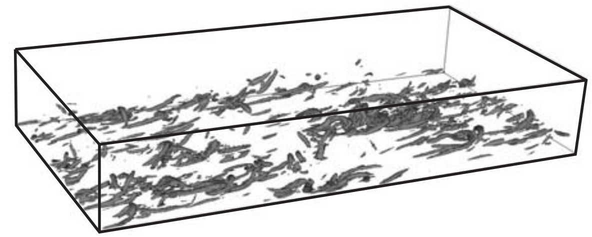


- Transient optimization and control problems are increasingly important:
  - Steady-state solutions do not capture critical physics: aeroacoustics, combustion instabilities, bluff-body wakes, . . .
  - Next generation systems will use *active* design/control techniques.
- Algorithmic Challenges:
  - Complex geometries
  - Unsteady flow physics
  - Localized, broadband physics
  - Gradient evaluation
  - Storage of time-history
  - Complex problem setup
  - Large-scale space-time problems

Transient PDE Constrained Optimization







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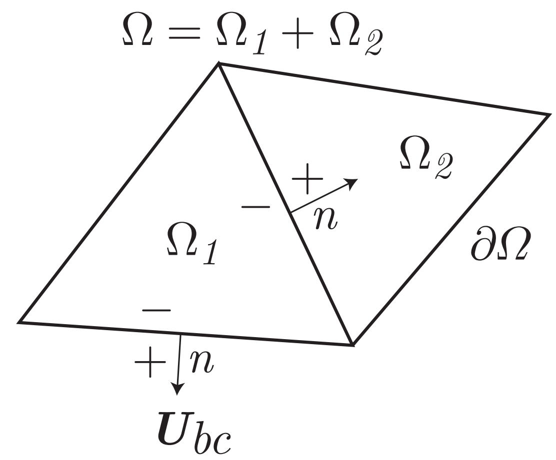
- DG-OPT
  - unstructured meshes.
  - high accuracy, low-dissipation.
  - multiscale / zonal models.
  - adjoint methods.
  - efficient I/O, checkpointing.
  - object-oriented software design.
  - parallel algorithms.

Discontinuous Galerkin Method

Strong form:



$$\boldsymbol{U}_{,t} + \boldsymbol{F}_{i,i} - \boldsymbol{F}^v_{i,i} = \mathbf{S}, \quad \text{in } \Omega$$

$$\boldsymbol{U}(\boldsymbol{x},0) = \boldsymbol{U}_0(\boldsymbol{x}), \quad \text{at } t = 0$$

and appropriate boundary conditions on $\partial\Omega$.

Partition Ω into N subdomains Ω_e.

$$\int_{\Omega_e} \left(\boldsymbol{W}^T \boldsymbol{U}_{,t} + \boldsymbol{W}^T_{,i}(\boldsymbol{F}^v_i - \boldsymbol{F}_i) \right) d\boldsymbol{x} + \int_{\partial\Omega_e} \boldsymbol{W}^T \left(\boldsymbol{F}_n - \boldsymbol{F}^v_n \right) d\boldsymbol{s} = \int_{\Omega_e} \boldsymbol{W}^T \mathbf{S}\, d\boldsymbol{s}$$

Introduce numerical fluxes $\boldsymbol{F}_n(\boldsymbol{U}) \rightarrow \widehat{\boldsymbol{F}}_n(\boldsymbol{U}^-, \boldsymbol{U}^+)$ and sum over all elements

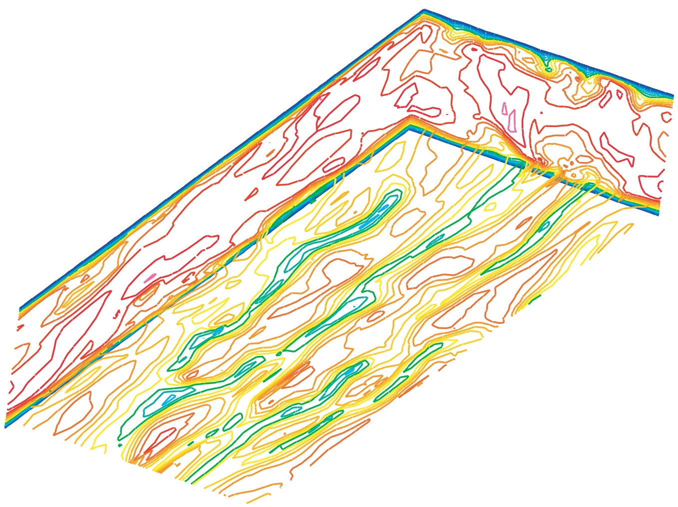
$$\sum_{e=1}^{N} \int_{\Omega_e} \left(\boldsymbol{W}^T \boldsymbol{U}_{,t} + \boldsymbol{W}^T_{,i}(\boldsymbol{F}^v_i - \boldsymbol{F}_i) \right) d\boldsymbol{x} \quad +$$

$$\sum_{e=1}^{N} \int_{\partial\Omega_e} \boldsymbol{W}^T \left(\widehat{\boldsymbol{F}}_n(\boldsymbol{U}^-, \boldsymbol{U}^+) - \widehat{\boldsymbol{F}}^v_n(\boldsymbol{U}^-, \boldsymbol{U}^+) \right) d\boldsymbol{s} \quad = \quad \sum_{e=1}^{N} \int_{\Omega_e} \boldsymbol{W}^T \mathbf{S}\, d\boldsymbol{s} \quad \forall \boldsymbol{W} \in \mathcal{V}$$

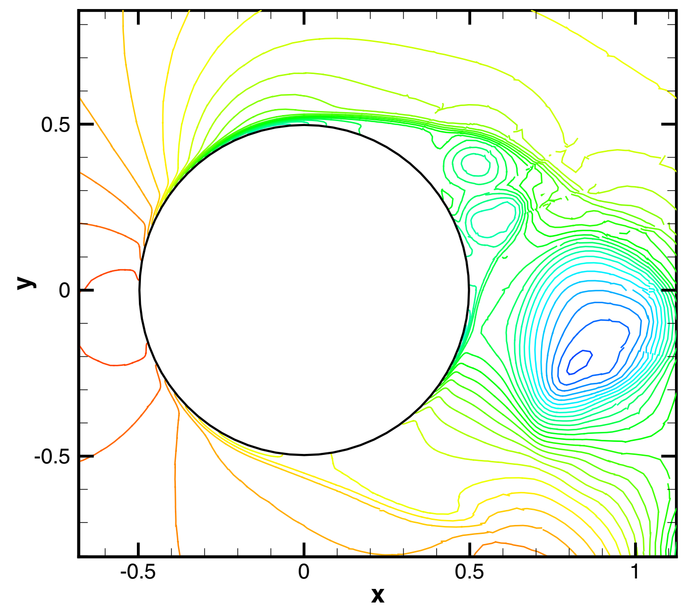
Benefits: High accuracy, unstructured, local *hp*-refinement, local conservation, …

Status of DGM Prototype Code

- Arbitrarily high-order discontinuous Galerkin spatial discretization,
- Explicit RK methods, implicit **Trilinos** implementation underway…
- LES-VMS approach for element-by-element subgrid-scale modeling
- Supports **multifidelity** and **multiscale** models
- Already validated for turbulent channel flow, bluff body wakes underway …



with Srinivas Ramakrishnan (Rice)



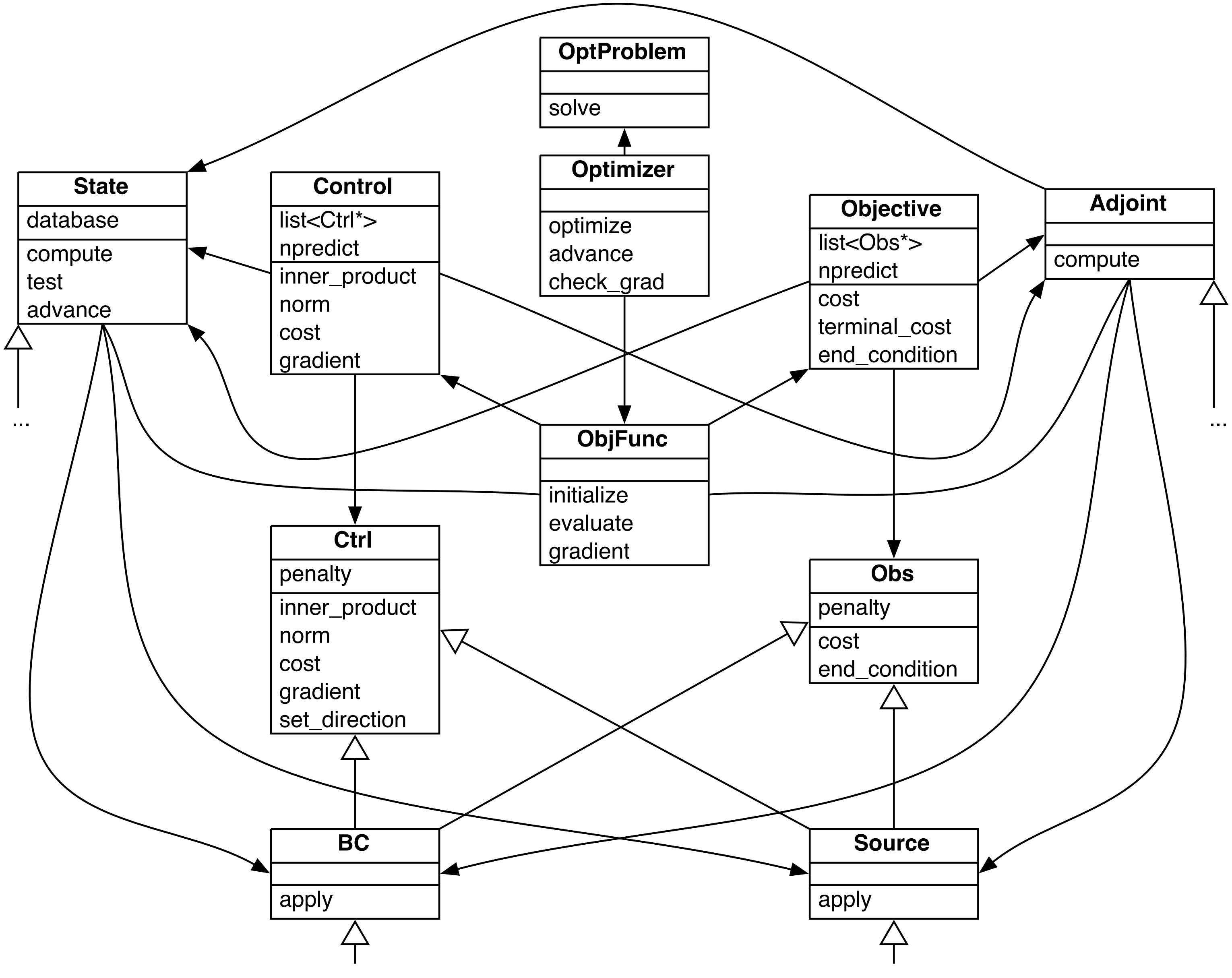
with Matt Barone (9115)

DG + Optimization: DG-OPT

Adjoint-based Gradient Method

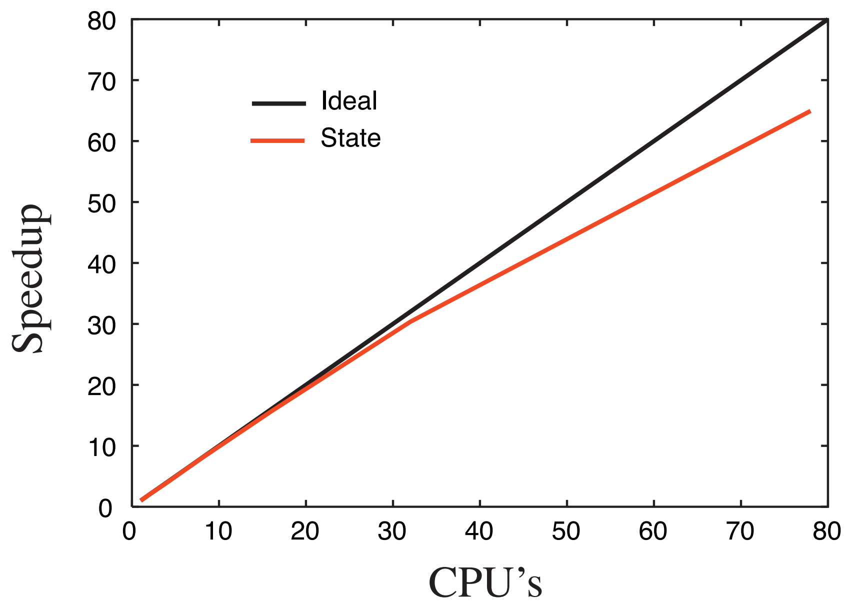
- Continuous adjoint formulation in space:
  - Adjoint PDEs are discretized using DG, similar to State equations.
  - Allows for accurate, stable, discretizations of both state and adjoint.
  - Enables different resolutions to be used for state and adjoint.
  - Obviates difficulties with non differentiable numerical fluxes and limiters
  - Provides insight into the physics of sensitivity systems and boundary conditions.
- Discrete adjoint in time: Runge-Kutta, Backward Euler, Crank-Nicholson
- Adjoint implemented for: Advection-Diffusion, Burgers, Wave, Euler, and Navier-Stokes
- Future work will take advantage of Sandia's DAKOTA and MOOCHO optimization tools…
- Time-domain decomposition techniques are in progress (Bartlet, Collis, Heinkenschloss, van Bloemen Waanders, 2004)…
- Generic solver/optimization interface mimics mathematical formulation …

DG-OPT Framework Design

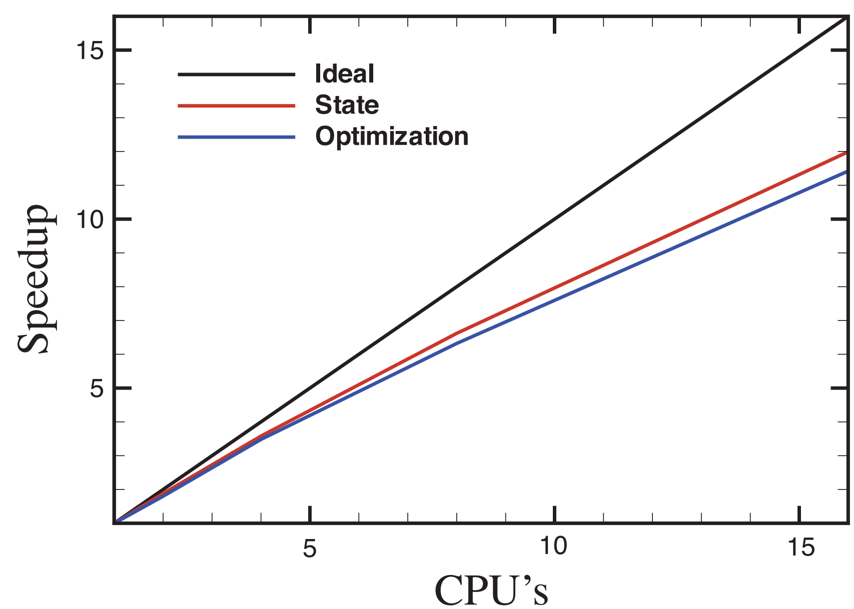


Preliminary Performance & Porting

- Demonstrated scaling of flow solver up to 80 processors, even on *modestly sized* two-dimensional problems ($\approx 10,000$ elements).
- Scaling of optimization problems same as flow solver, so far…
  (Note that optimization problem is small — only 576 elements!)



Parallel speedup of DGM Solver.



Parallel speedup of DGM Optimization.

- Ported to many Sandia/DOE platforms:
  Cplant, QT, RedStorm prototypes, Rogue/Renegade, Liberty/Shasta

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Example: Cylinder Wake Control

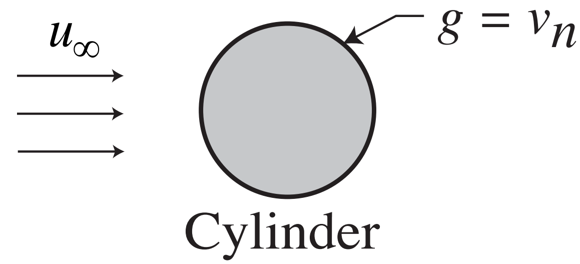
$$\min_{g \in \mathcal{G}} \mathcal{J}(g)$$

where

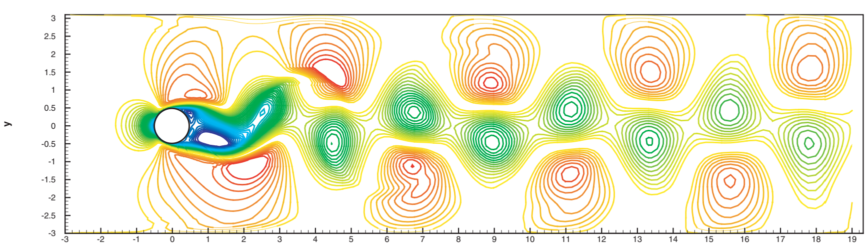
$$\mathcal{J}(g) = \frac{1}{2}\int_{\Omega_o}\int_0^T \left|\boldsymbol{u} - \hat{\boldsymbol{u}}\right|^2 d\Omega dt + \frac{\alpha}{2}\int_{\Gamma_w}\int_0^T g^2 d\Gamma dt$$

such that

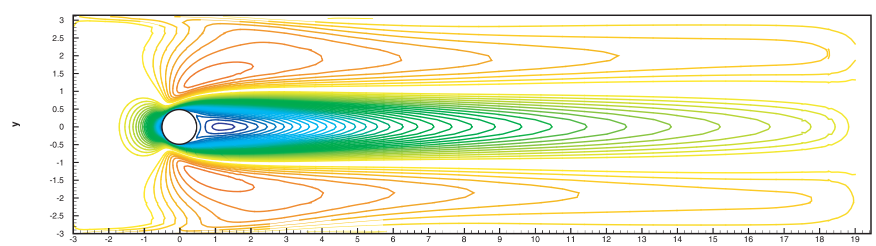
$$\mathcal{N}(\boldsymbol{u}, g) = 0 \quad \text{(Navier–Stokes)}$$



- $Re = 100$, $M_\infty = 0.5$.
- DG: $N_e = 576$ quads with $p = 4$
- RK4: $N_t = 2,000$, $\Delta t = 0.0015$.
- Consider both *unsteady* and *steady* suction/blowing.



Uncontrolled ρu at $Re = 100$.

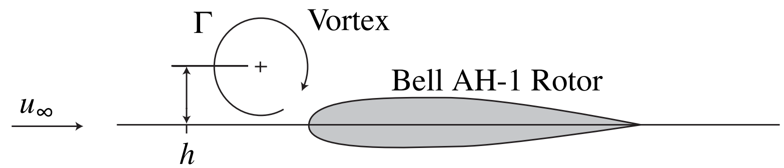


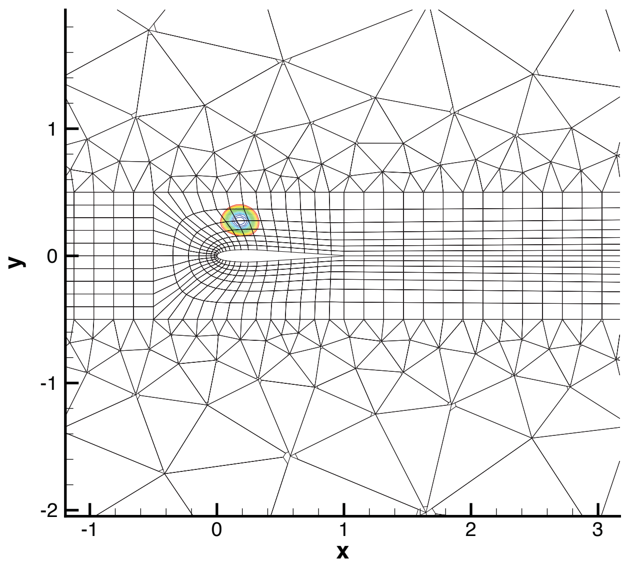
$\hat{\boldsymbol{u}}$: uncontrolled ρu at $Re = 20$

Multimodel & Multifidelity Optimization

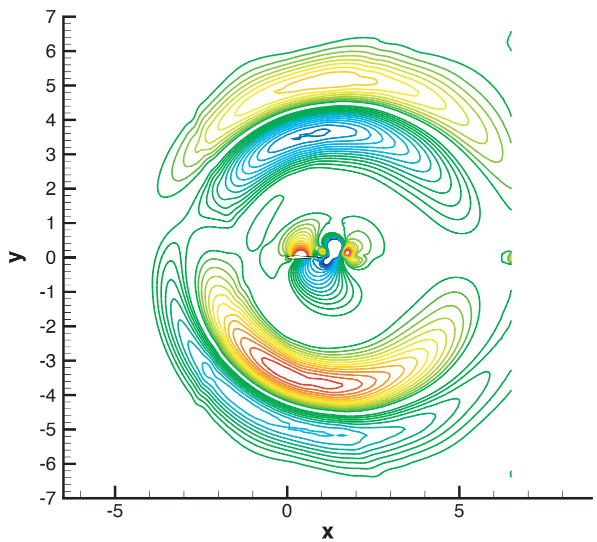
Bell AH-1 Blade-Vortex Interaction

- Conditions: $Re = 100$, $M_\infty = 0.3$
- Vortex: location $(x_0, y_0) = (-6, 1/4)$, core radius $R_c = 0.15$, maximum velocity $v_{\theta\,\max} = 1/2$.

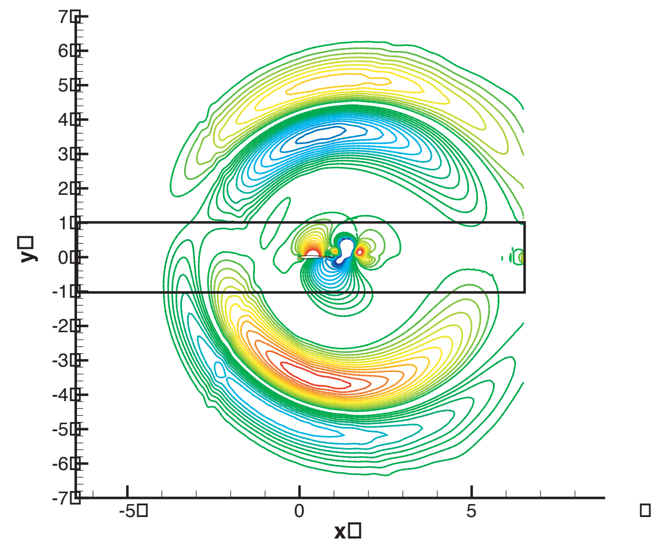




Mesh + Vorticity



Scattered Pressure:
Navier–Stokes



Scattered Pressure:
Navier-Stokes +
Linearized Euler

Optimization results for multimodel/multifidelity models have been obtained!

(95% reduction in acoustic energy!)

Multiscale Methods

- Many Sandia applications exhibit nonlinear multiscale behavior:
  - strong-shock Z-pinch physics,
  - turbulent reacting flows in pool fires,
  - turbulent flows for reentry vehicles,
  - failure of metallic microcomponents in weapons systems, ...
- Two primary classes of multiscale applications:
  1. Same continuum model holds at all scales → computational resources.
  2. Atomistic/molecular simulations required for small scales → requires coupling to continuum level.
- Organized interdisciplinary research team:

  Pavel Bochev (9214), Mark Christon (9231), Scott Collis (9211), Rich Lehoucq (9214), Alex Slepoy (9235), John Shadid (9233), and Greg Wagner (8752)
- Forming external collaborations:

  Tom Hughes (UT-Austin), Donald Estep (Colorado State), Max Gunzburger (Florida State)
- Application areas:

  fluid dynamics, shock hydrodynamics, solid mechanics, and materials science.

General Multiscale Mathematical Framework

- Basic foundation: Variational Multiscale (VMS) Method (Hughes et al., 2000)
- Identified common issues in multiscale applications:
  - *Scale representation,*
  - *Scale separation,*
  - *Interscale communication.*
    - Coupling of different models and physics at different scales,
    - Subgrid scale models,
    - Creation/destruction of information at interfaces…

  Key Idea: Combine VMS with DG $\rightarrow$ local VMS (ℓVMS)
  - Use VMS formulation within spatial regions,
  - Generalize the idea of *numerical fluxes* to *interscale transfer operators*,
  - Use weak coupling of *interscale transfer operators* over space-time interfaces
  - Within space-time regions, subgrid-scale modeling via VMS
- LDRD idea accepted for full proposal…
- MICS-DOE Multiscale whitepaper in progress…

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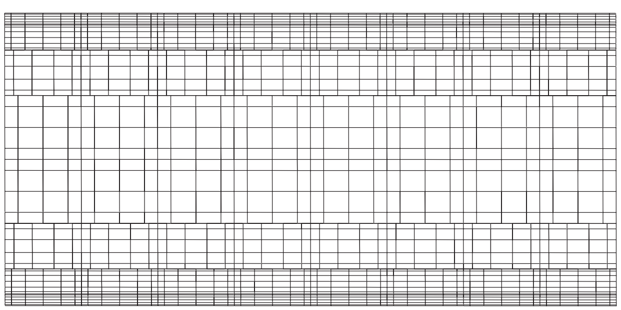
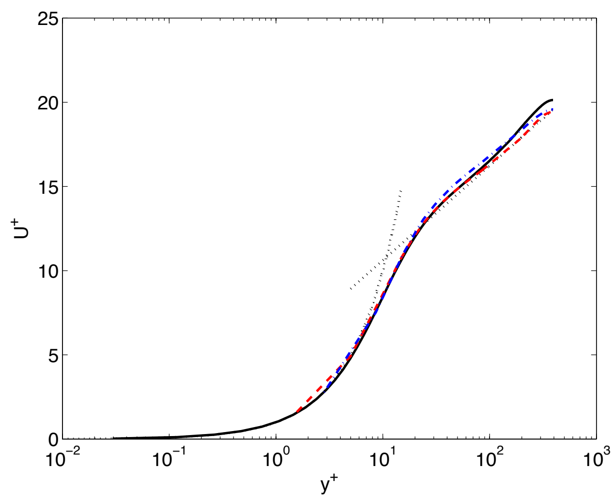
Example: ℓVMS for Turbulent Channel Flow

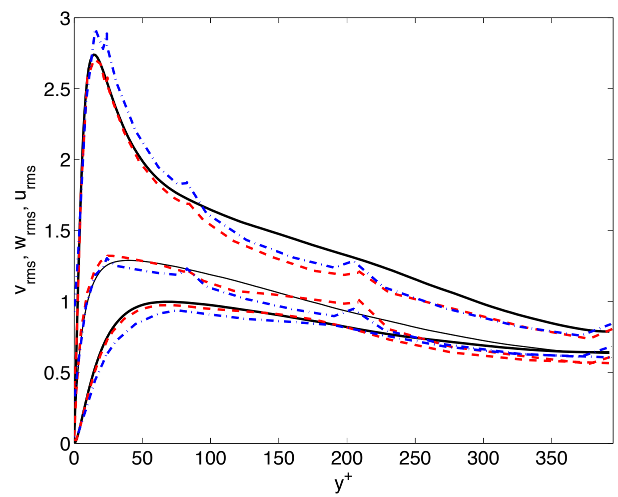
- Fully developed turbulent channel flow: $Re_\tau = 395$, $M = 0.3$
- Variable p-refinement near walls: $p = 6, 6, 5, 4, 4, 5, 6, 6$
- VMS modeling on small scales with 50/50 partition, variable small-scale space.
- ℓVMS rovides extensive flexibility (variable resolution and models)
- Note excellent agreement with DNS, especially in near-wall region.



Crossflow (x-y) grid



Mean velocity



RMS Velocities

——— DNS; —·— $8 \times 8 \times 18$ with $p = 4$;
- - - - $8 \times 8 \times 18$ with $p = \{6, 6, 5, 4, 4, 5, 6, 6\}$

Internal Impact: 2003–2004

- Submitted MICS proposal:
  Multiscale Modeling and Simulation (with Mark Christon)

- Submitted 4 LDRD ideas:
  - *Mathematical Framework for Multiscale Science and Engineering: The Variational Multiscale Method and Interscale Transfer Operators*
    (with Pavel Bochev, Mark Christon, John Shadid, Alex Slepoy, and Greg Wagner.)
  - *Multiresolution Limiters for High-Order Methods* (with Mark Christon)
  - *Adjoints of Adjoints for Optimal and Robust Sensor System Design*
  - *Adjoint Methods for Receptivity Prediction in High-Speed Flows*
    (with David Kuntz)

- Working toward incorporating DG technology into Sandia simulation tools: Premo (SIERRA), Charon (NEVADA).

- Recruited summer student: Lucas Wilcox (Brown University) to work on adjoint based error estimation.

External Impact: 2003–2004

- University collaborations: TJR Hughes (UT-Austin), M Heinkenschloss (Rice), G Chen (Rice), S Ramakrishnan (Rice)
- Publications/Presentations:
  - 5 journal articles (2 published, 1 accepted, 2 in-review),
  - 4 conference papers (1 invited),
  - 2 abstracts,
  - 3 conference presentations (1 invited).
- Reviewer:

  Journal of Fluid Mechanics (1), Physics of Fluids (2), Computer Methods in Applied Mechanics and Engineering (1), AIAA Journal (1), Encyclopedia of Computational Mechanics (1), Journal of Turbulence (1)
- Technical societies:
  - AIAA Working Group: *Algorithms and Architectures for Active Flow Control*
  - AIAA Aeroacoustics Technical Committee
  - Session Chair: *42nd AIAA Aerospace Sciences Meeting and Exhibit, Aeroacoustics: Modeling and Mechanisms*
  - Forum Organizer: *4th ASME/JSEM Joint Fluids Engineering Conference*

Closing Comments and Future Directions

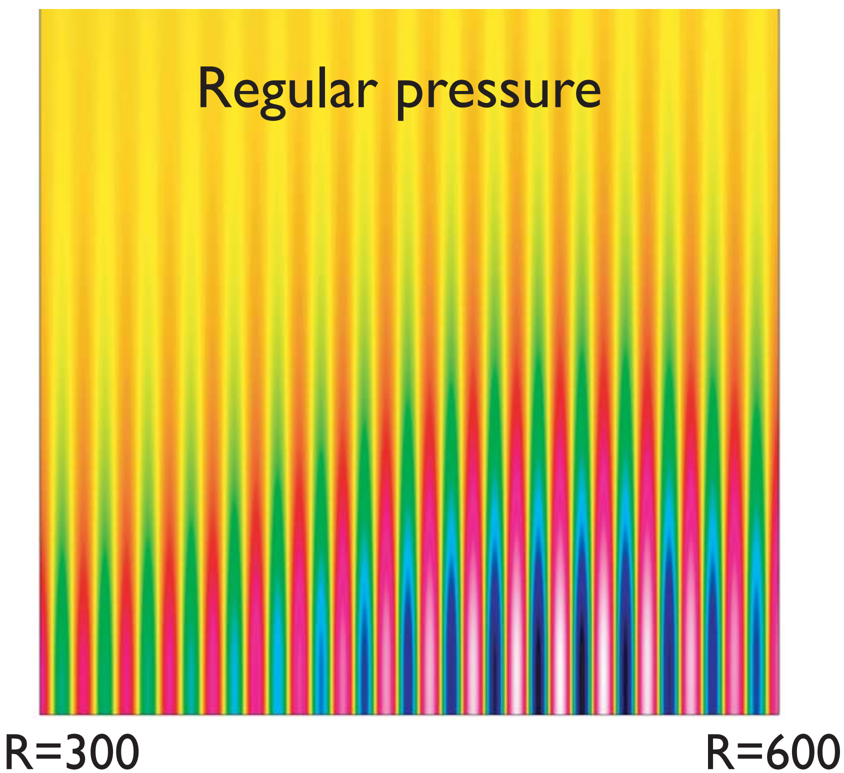
- DG-OPT Simulation framework is operational for transient, multimodel, multiscale optimization problems.
- Emphasis this year on spatial discretization, multimodel capability, and optimization framework.
- Future work will apply DG-OPT to key Sandia applications:
  - ASC $\rightarrow$ optimal *control/design* applied to jet-in-crossflow.
  - DHS $\rightarrow$ optimal *control/design* of HVAC systems for bio/chem remediation.
- Important near-term goal: *Trilinos* (Epetra/NOX) for implicit time advancement.
- Key areas for further research:
  - Link multiscale formulation with ROM for use in optimization,
  - Multimodel and multifidelty methods for optimization,
  - Move DG-OPT technology to ASC frameworks.

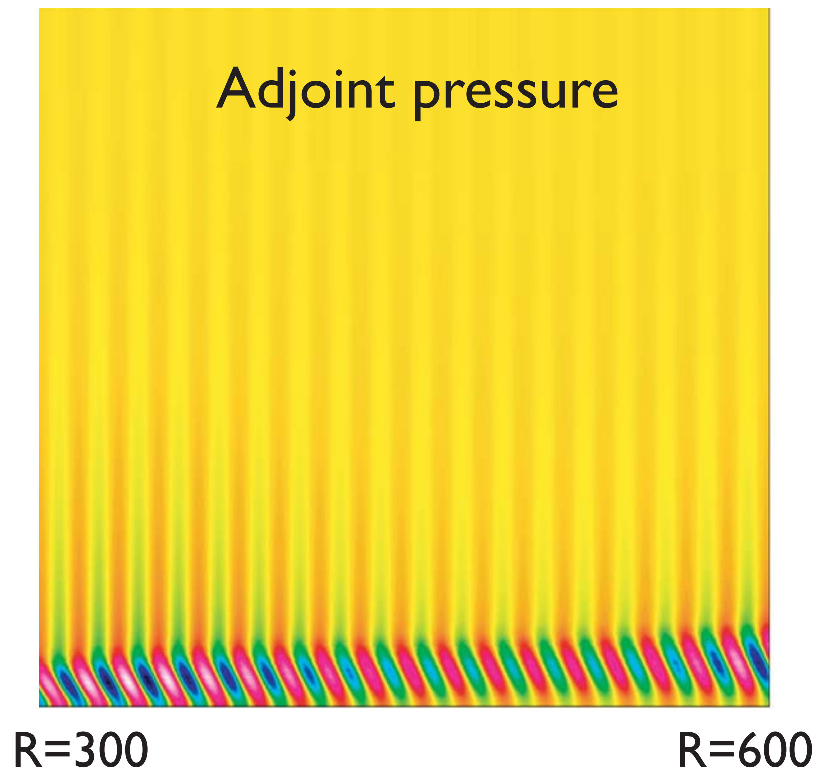
Extra Slides

Eigensolutions

Blasius boundary layer, F=150

- Adjoint grows upstream
- Adjoint is localized near the wall, with higher spatial gradients
- Adjoint wavelength is approximately the same as the Tollmien-Schlichting wavelength

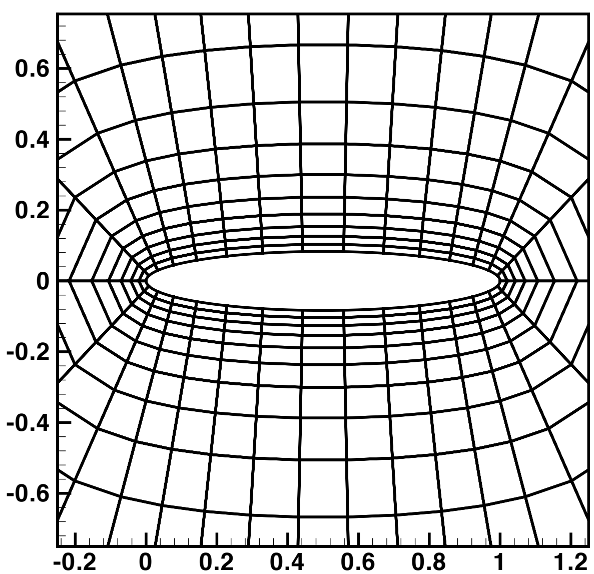




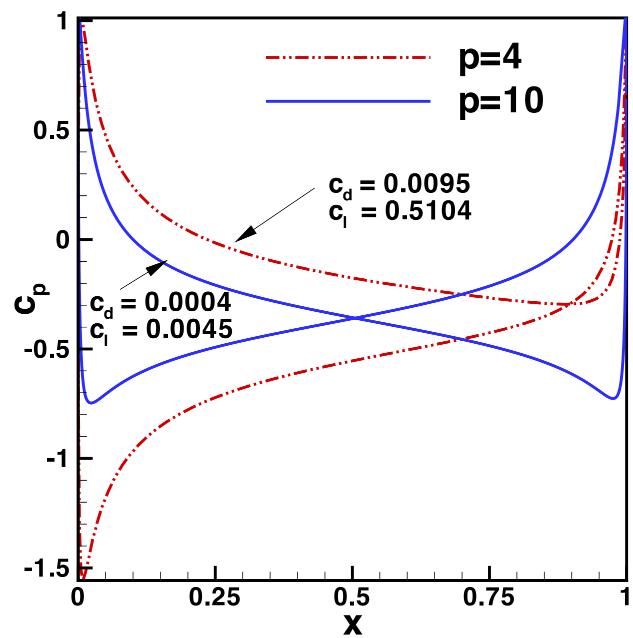
Numerical Dissipation: Inclined Ellipse

$$AR = 6, M_\infty = 0.2, \alpha = 6°$$

- Test case originally proposed and studied by T. Pulliam (1990).
- Solution with zero-circulation initial condition should remain non-lifting.
- Numerical dissipation generates vorticity which leads to lift.



Element mesh



Pressure coefficient

- High-order DG solution is nearly symmetric (i.e. non-lifting).

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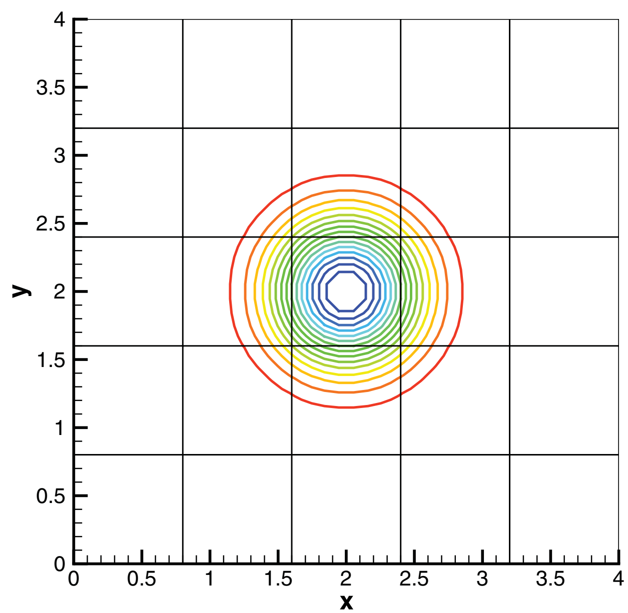
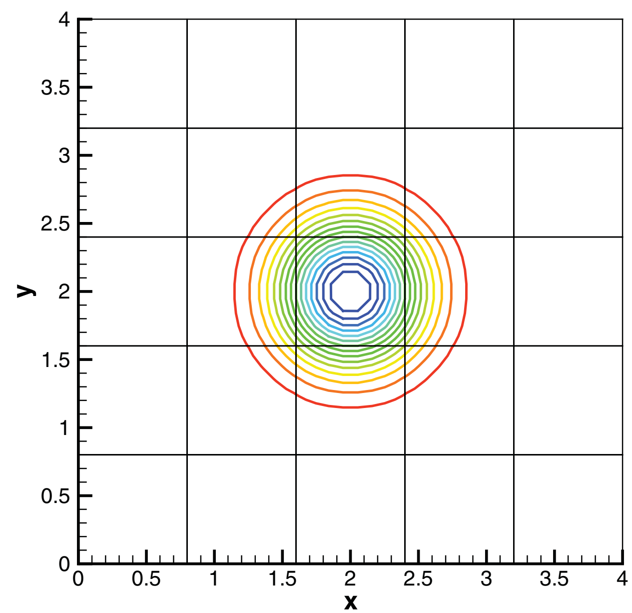
Numerical Dissipation: Vortex Propagation

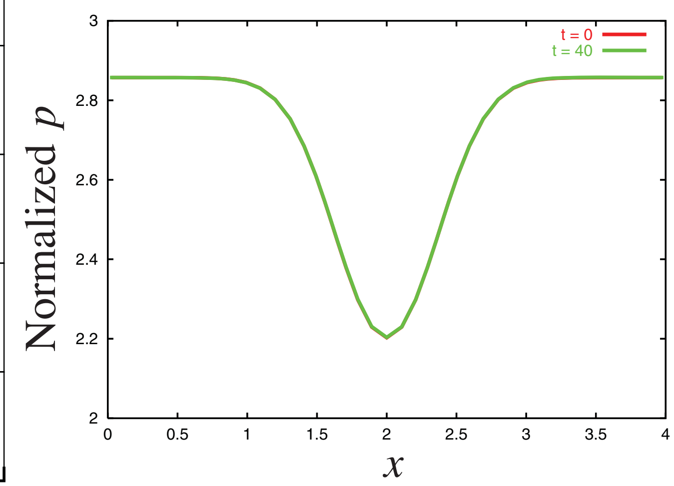
- Conditions: inviscid, $M_\infty = 0.3$ mean flow.
- Vortex core diameter $D_c = 1.0$, maximum velocity $v_{\theta\,\max} = 0.5$.
- 5×5 element array, $p = 5$ elements, periodic boundaries.



Initial condition



$t = 40$



Pressure profiles

- Negligible error to graphical accuracy.
- Analysis of Hu *et al*. (1999) verifies low dissipation and dispersion of DG methods.