

CFD, PDEs, and HPC

A Thirty Year Perspective

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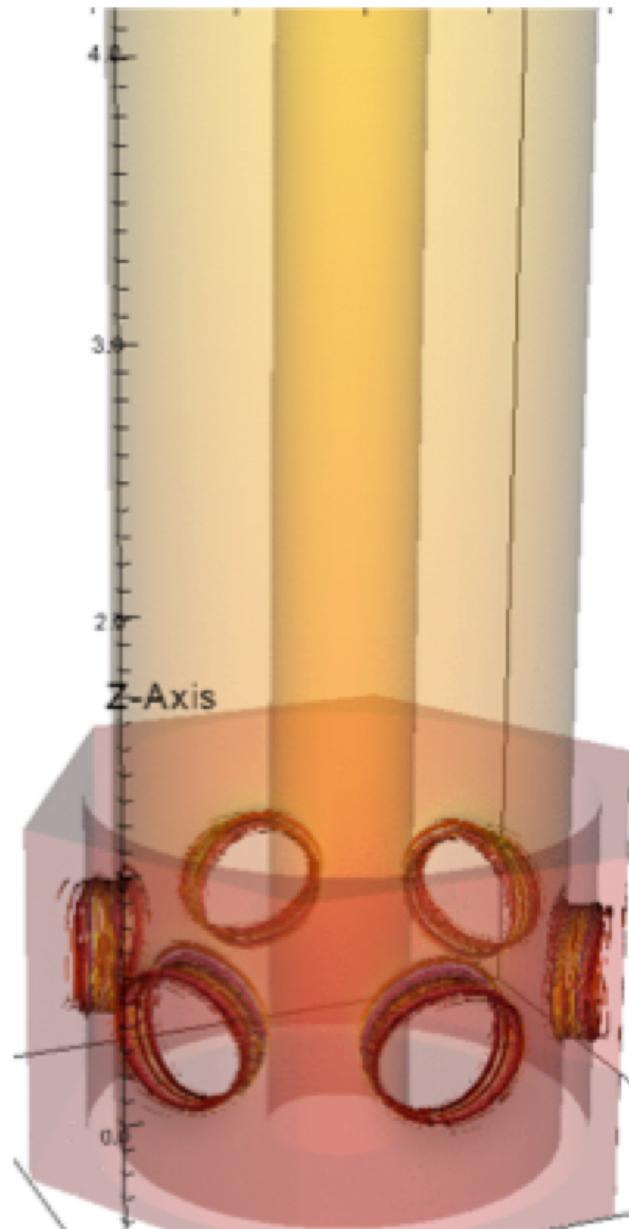
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Martin Schmitt

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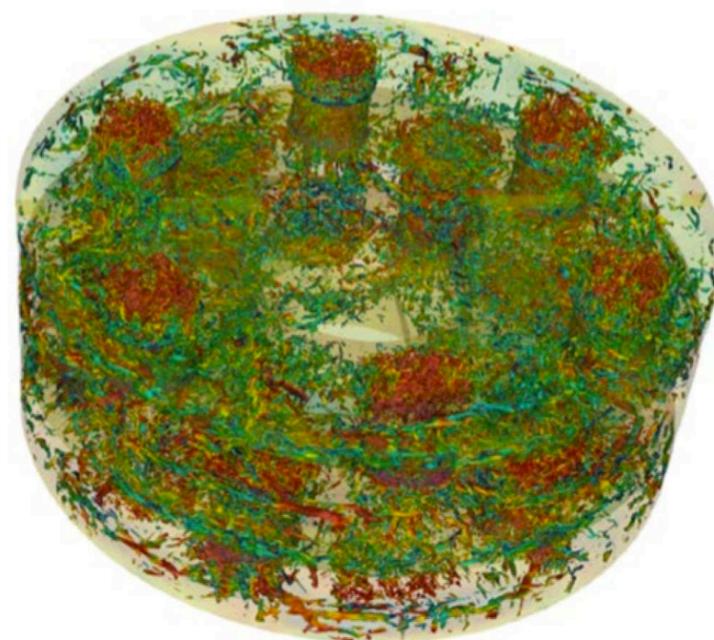
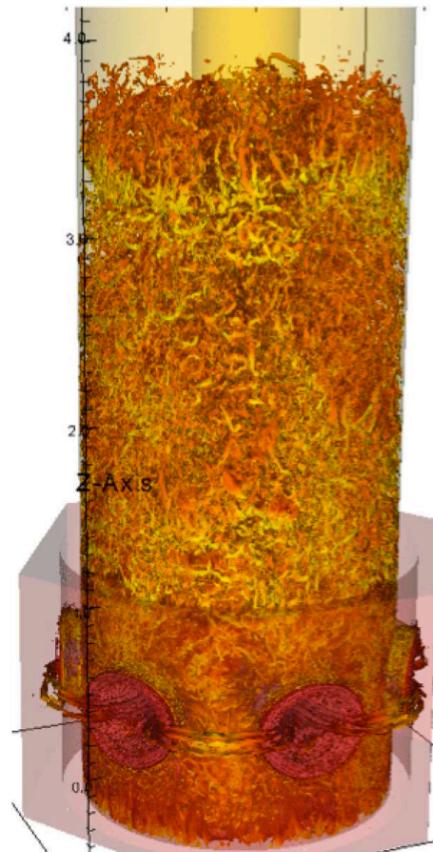
Active users group (> 250)



Turbulence in a heat-exchanger inlet.

Industrial Example

- 12 hour turnaround for result on the left:
 - 6 hours to mesh, 6 hours to run on 16K cores
- 3 Days for result on the right (mostly meshing...)



Outline

- *Turbulence*
- *PDE discretization and solve strategies*
- *HPC*

Incompressible Navier-Stokes Equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u}$$
$$\nabla \cdot \mathbf{u} = 0$$

■ Key algorithmic / architectural issues:

- Unsteady evolution implies many timesteps, significant reuse of preconditioners, data partitioning, etc.
- $\text{div } \mathbf{u} = 0$ implies ***long-range global coupling at each timestep***
 - iterative solvers
 - communication intensive
- Small dissipation → large number of scales → large number of gridpoints for high Reynolds number Re

Navier-Stokes Time Advancement

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u} \\ \nabla \cdot \mathbf{u} &= 0\end{aligned}$$

- Nonlinear term: *explicit*
 - k th-order backward difference formula / extrapolation ($k = 2$ or 3)
 - k th-order characteristics (Pironneau '82, MPR '90)
- Linear Stokes problem: pressure/viscous decoupling:
 - 3 Helmholtz solves for velocity (“easy” w/ Jacobi-precond.CG)
 - **Poisson equation for pressure** (*computationally dominant*)

Fluid Dynamics and Computing: Scale Complexity

- Fluid dynamics governs a broad range of physical phenomena governing our daily lives: vascular flow, transportation, energy production and consumption, weather (atmosphere and ocean), astrophysics, ...
- The majority of fluid flow is **turbulent**
 - A broad range of scales of motion with nonlinear interaction.
 - Sensitive to initial conditions (and other forcing) – Lorenz '63
 - **Nonrepeatable** 😞
- However, in the mean, many flows are repeatable and predictable.
 - Reynolds-Averaged Navier-Stokes (RANS) equations are excellent models for computing the predictable cases – 10^5 x cheaper than LES
- The trick is to know which cases are repeatable and which are not.
 - Unfortunately, there is no theory to say which cases are amenable to RANS approaches, and which are not.

Example of Sensitivity: ANL MAX Experimental Validation Study

- Argonne has constructed a highly instrumented experiment (MAX) to provide detailed velocity and temperature data for code validation.
 - $1 \times 1 \times 1.68 \text{ m}^3$ mock-up of mixing in outlet plenum (SFR or VHTR)
 - PIV for velocity measurements
 - Fast thermal video imaging for temperature measurements

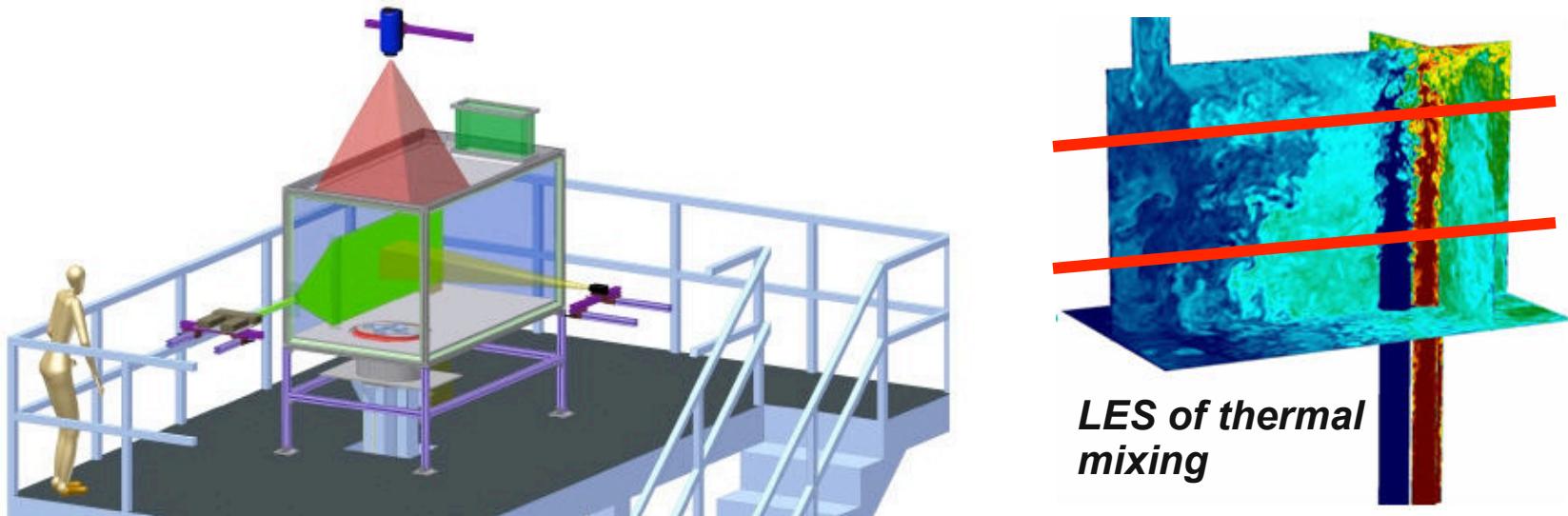
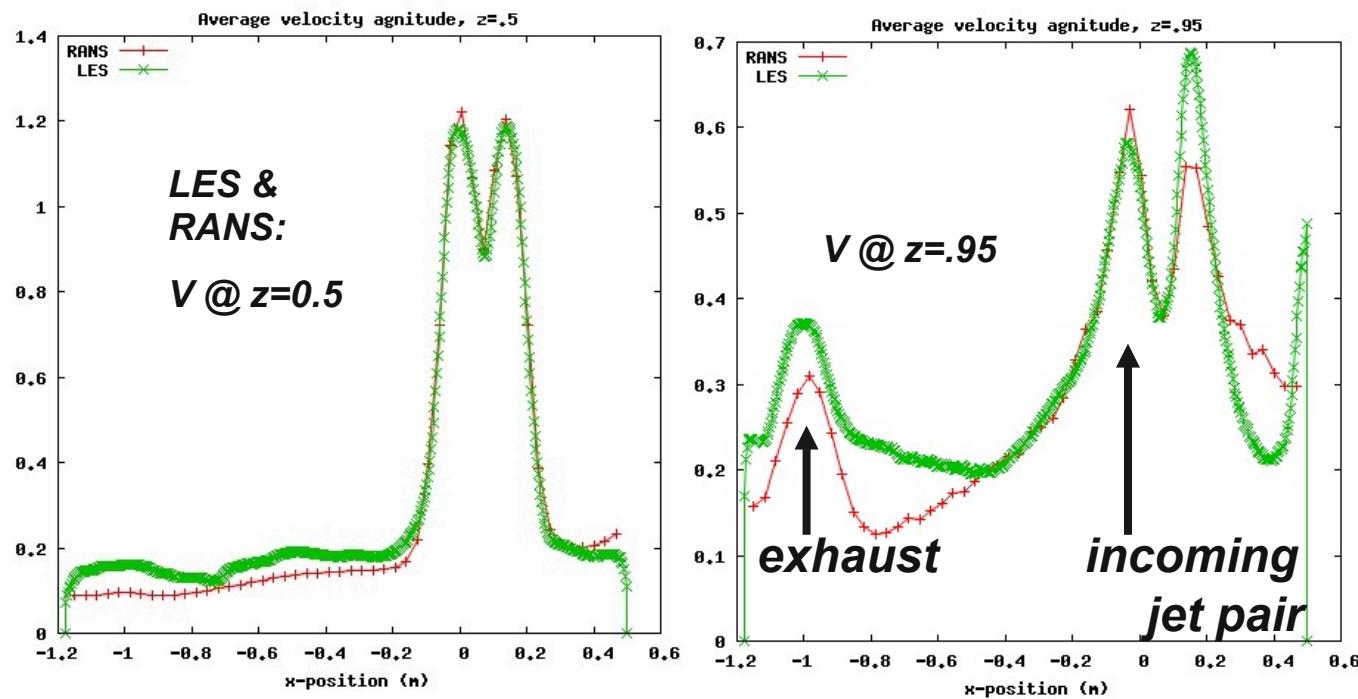


Figure 1. Apparatus for gas mixing experiments: Nd:YLF laser (left), infrared camera (top), PIV camera (right), and hexagonal flow channels (below).

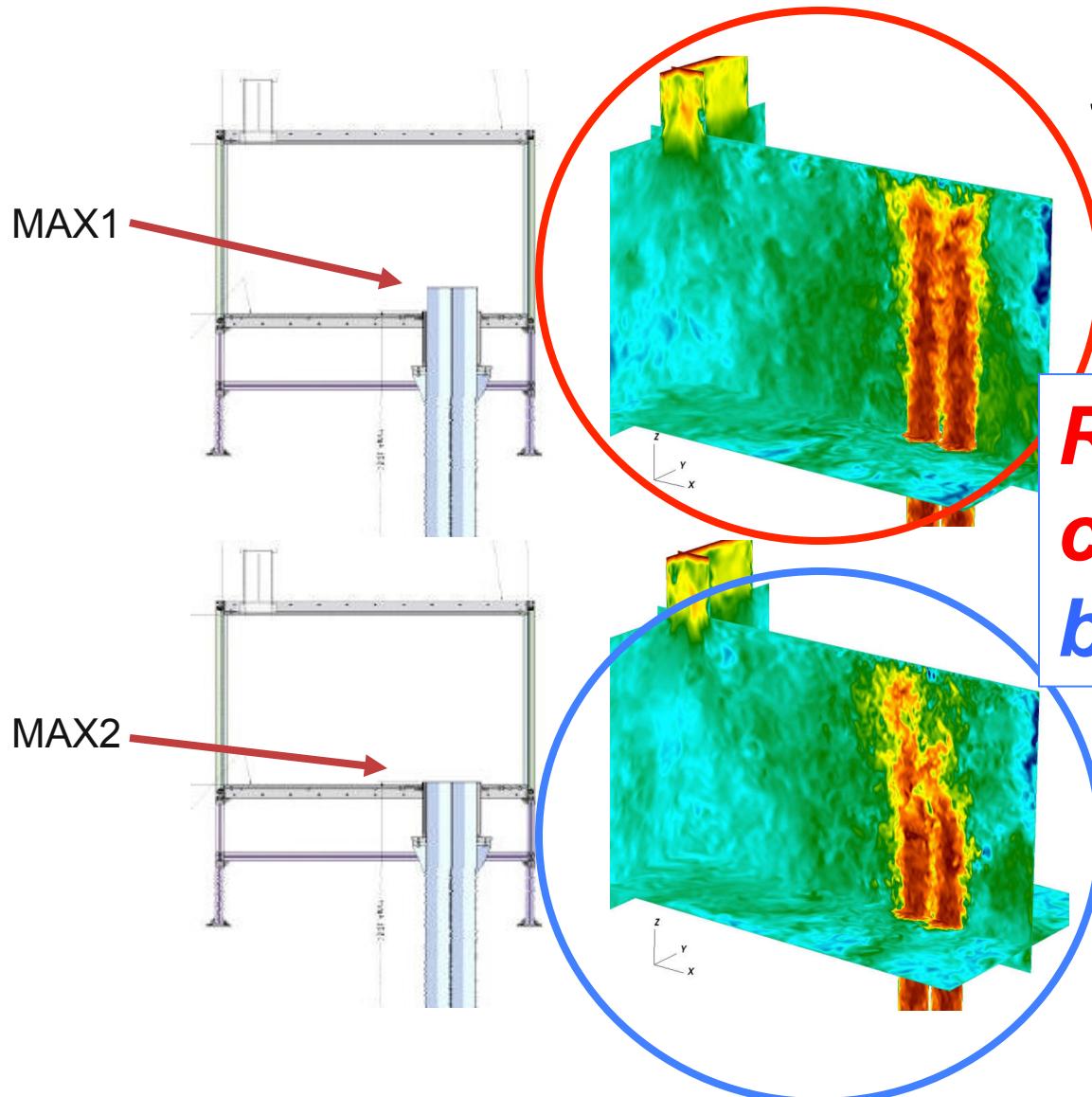
ANL MAX Experiment: LES / RANS Comparisons¹

- Time-averaged Nek5000 LES vs. Star-CD RANS velocity profiles at $(x,y,z) = (x,0,z)$, with $z=0.5$ m and $z=0.95$ m
- **RANS about $10^5 \times$ cheaper.**



¹ Merzari et al., *On the numerical simulation of thermal striping in the upper plenum of a fast reactor*, ICAPP (2010)

Major Difference in Behavior for Minor Design Change



Simulation Results:

- Small perturbation yields $O(1)$ change in jet behavior

Red case $10^4\times$ cheaper than blue case

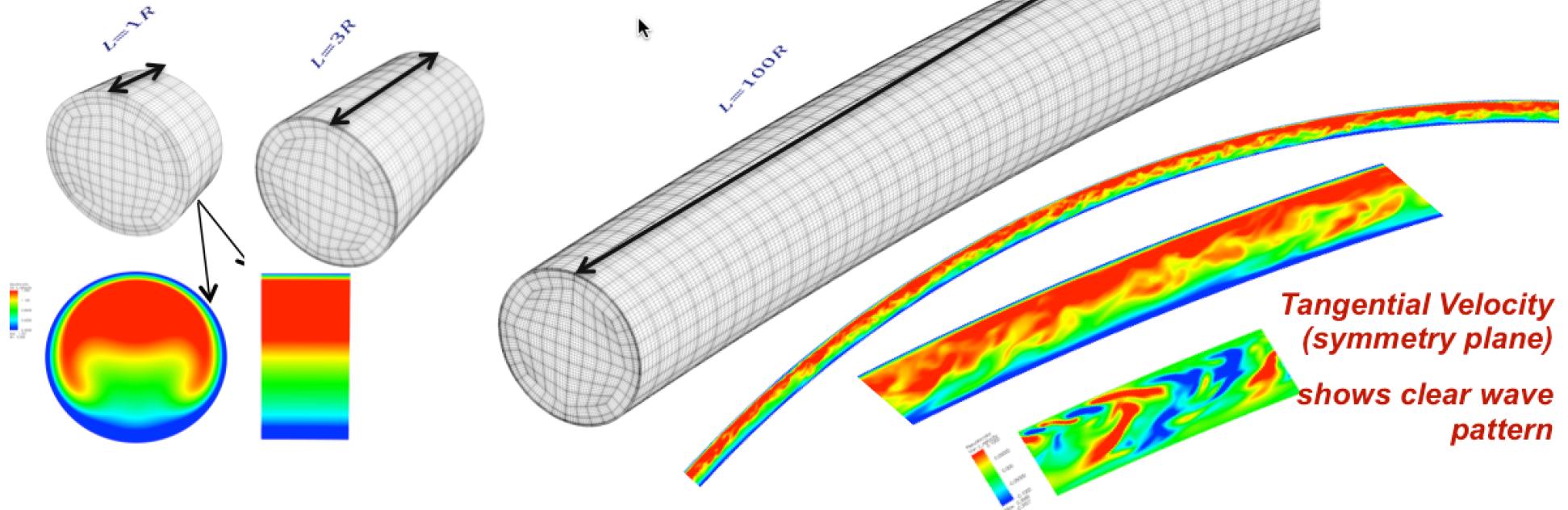
Visualization shows

change due to jet / cross-flow interaction

- MAX2 results NOT predicted by RANS

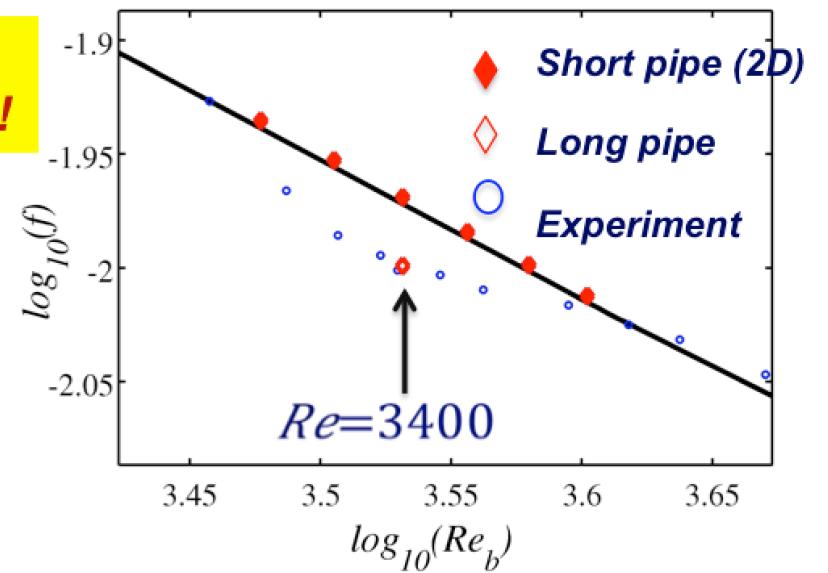
Sublaminar Drag in Curved Pipe Flow

— Noorani & Schlatter '12



- DNS results are being used to calibrate new RANS models in commercial engineering codes.

10% drag reduction!



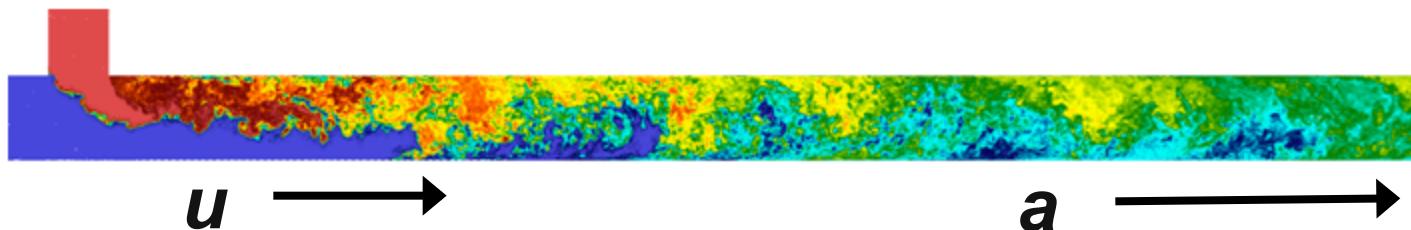
Fluid Dynamics and Computing: Scale Complexity (2)

- Fortunately, Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS) rely on very little modeling (none, in the case of DNS) and are therefore able to capture many features of turbulent flow.
- These approaches require simulation of a ***broad range of scales*** and their success is largely tied to that of parallel computing.
- Prior to the 80s, the majority of fluid flow simulations were 2D
 - *Definitely not turbulent!*
- A brief taxonomy gives some insight to the fluid dynamics computational landscape

Incompressible Navier-Stokes Equations

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$$\nabla \cdot \mathbf{u} = 0$$

- Physics: Low Mach-number flow:



- Interesting speed $u \ll$ sound speed, a (1000x)

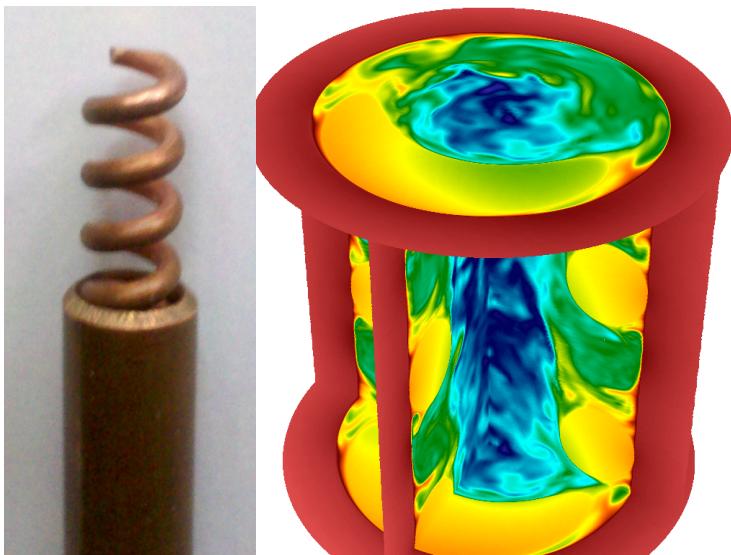
- Multiscale Math:

- Replace fast time-scale with an infinitely fast one and use optimal solvers to solve resulting elliptic problem: $\nabla^2 p = f$
- Architectural Influence: global coupling

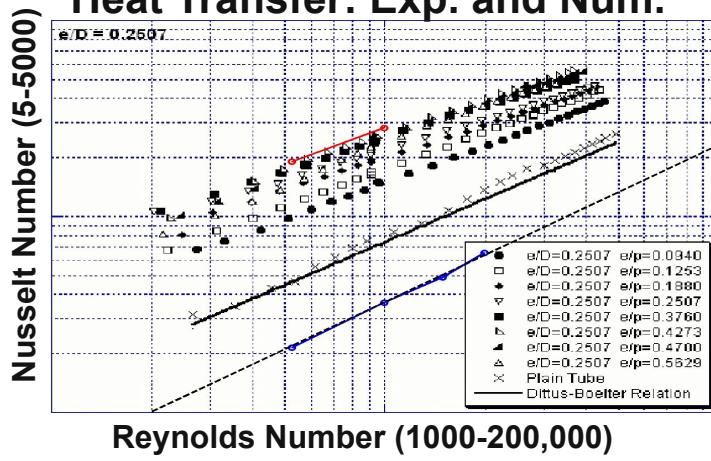
- Highly nonlinear & singularly perturbed – a huge range of scales

Some Turbulence Examples

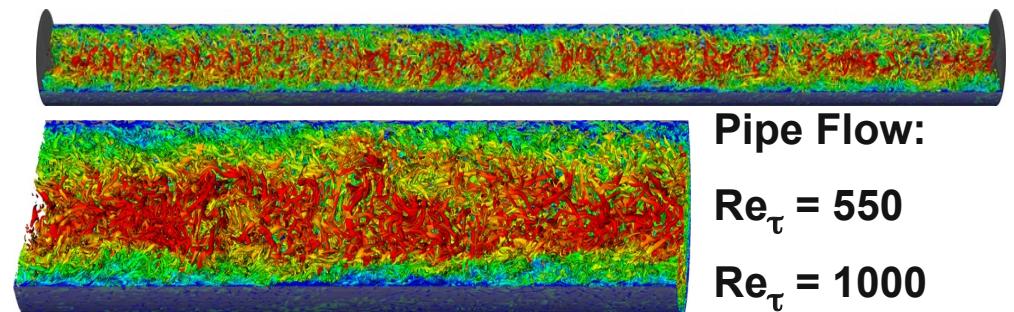
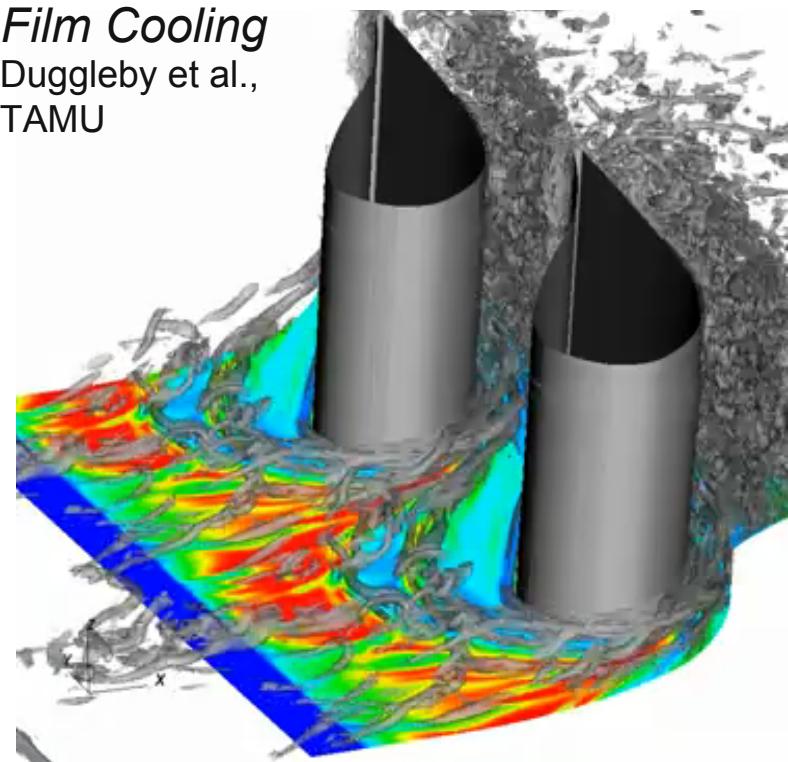
Optimizing Heat Transfer with Wire-Coil Inserts J. Collins, ANL



Heat Transfer: Exp. and Num.



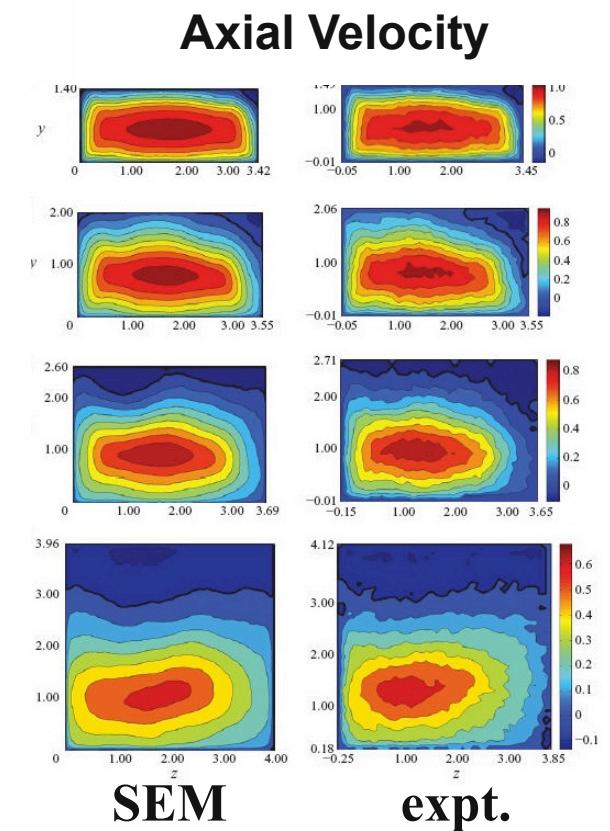
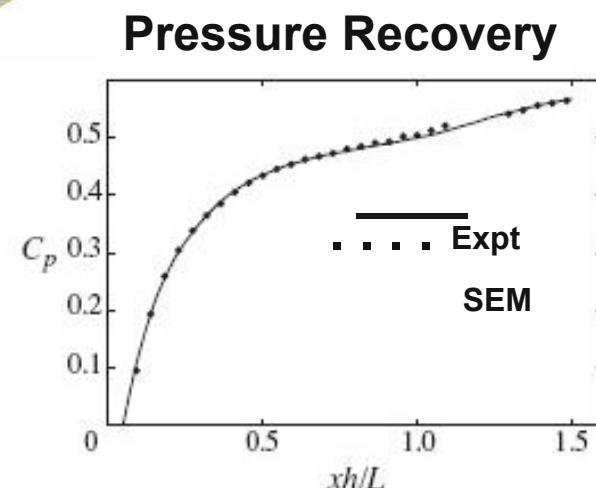
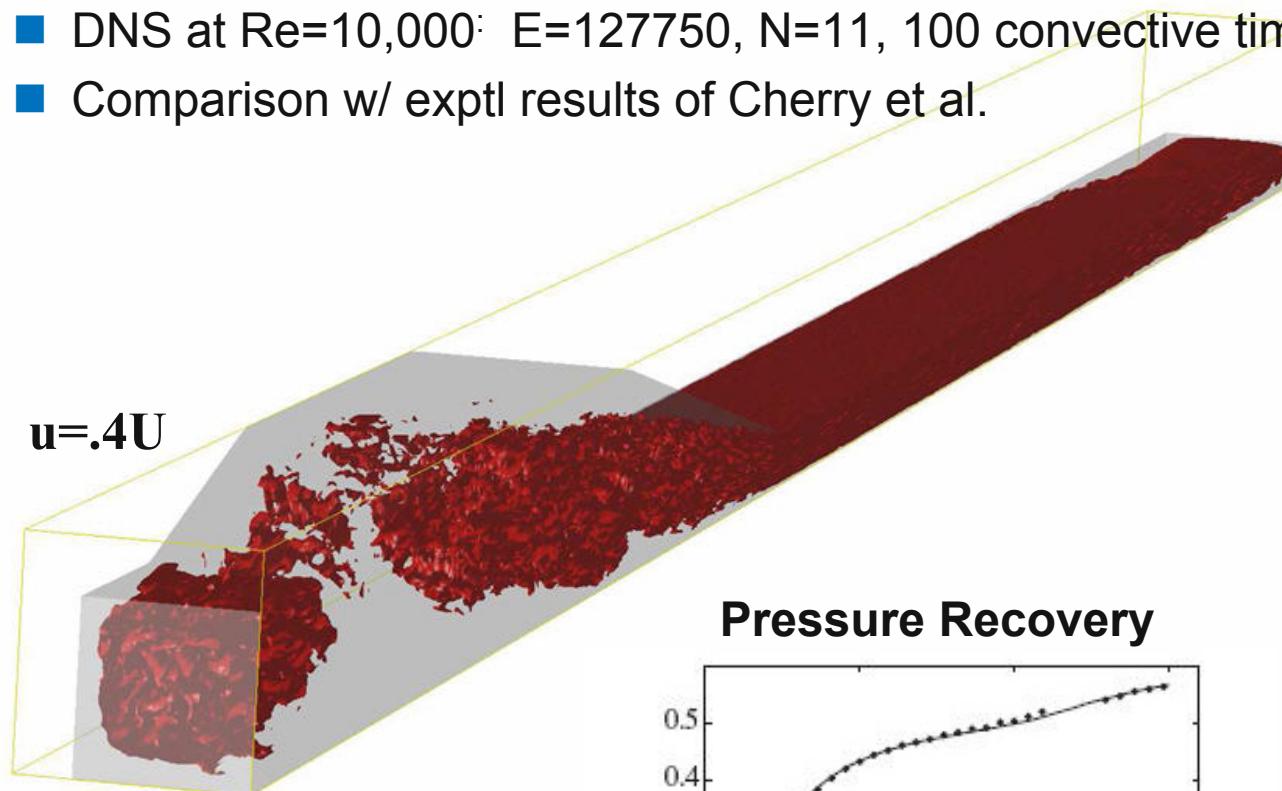
Film Cooling Duggleby et al., TAMU



Pipe Flow:
 $Re_\tau = 550$
 $Re_\tau = 1000$
G. El Khoury, KTH

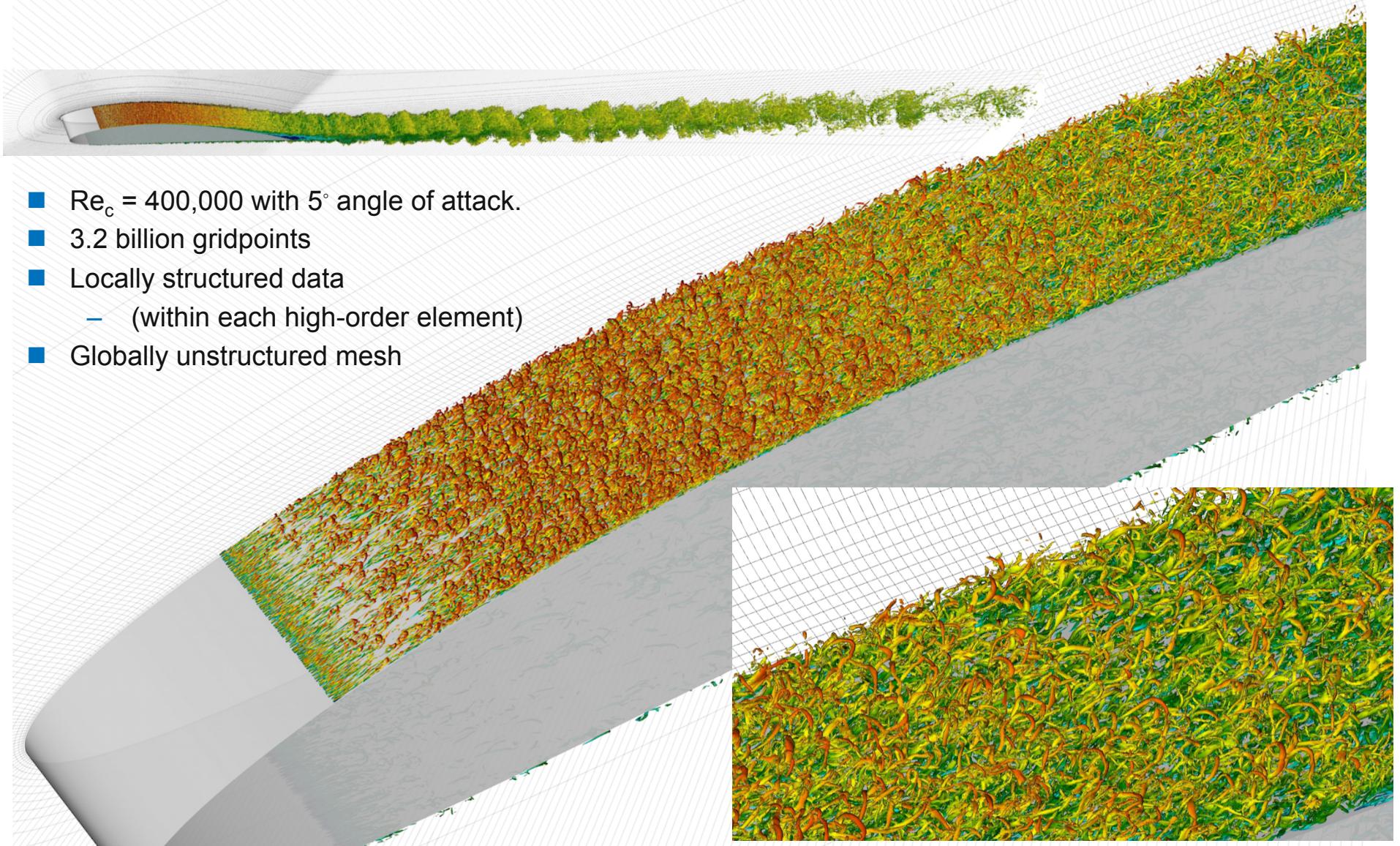
DNS Separation in an Asymmetric Diffuser

- Flow separation and recovery
- DNS at $Re=10,000$: $E=127750$, $N=11$, 100 convective time units
- Comparison w/ exptl results of Cherry et al.



DNS of Flow around a NACA4412 Wing Profile

Armin Hosseini et al. (KTH)

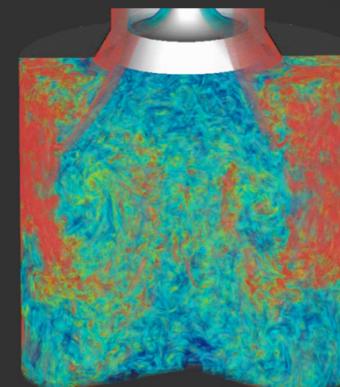
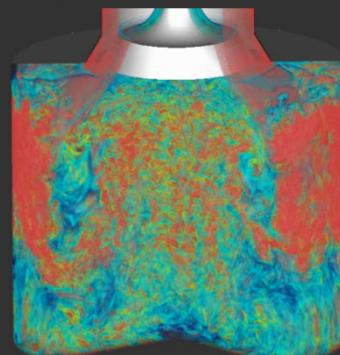
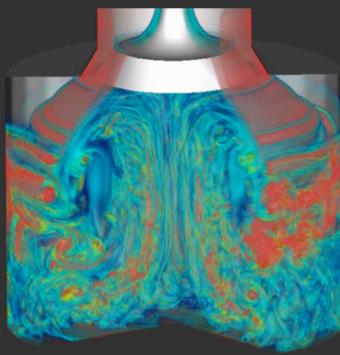
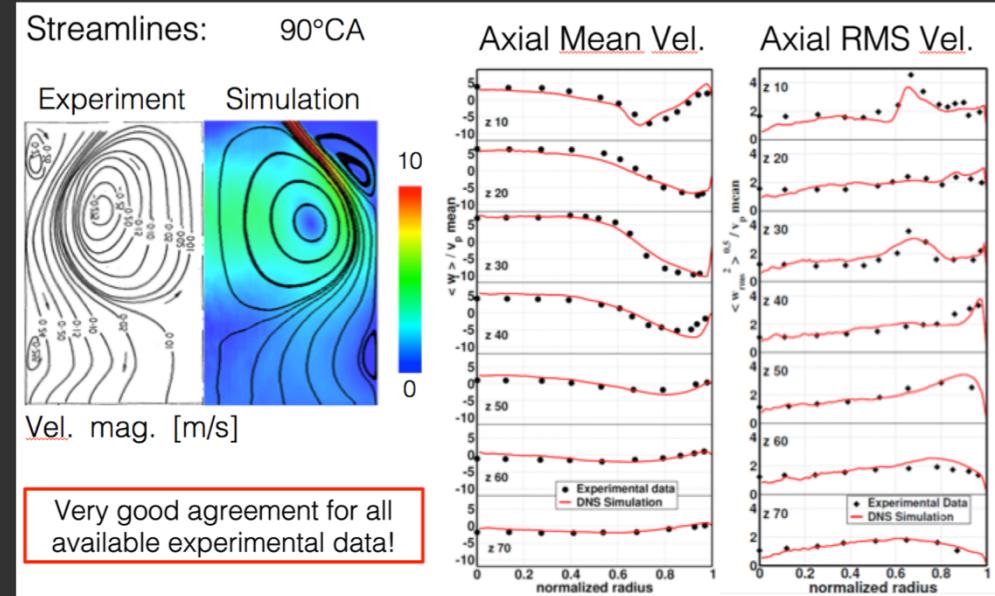
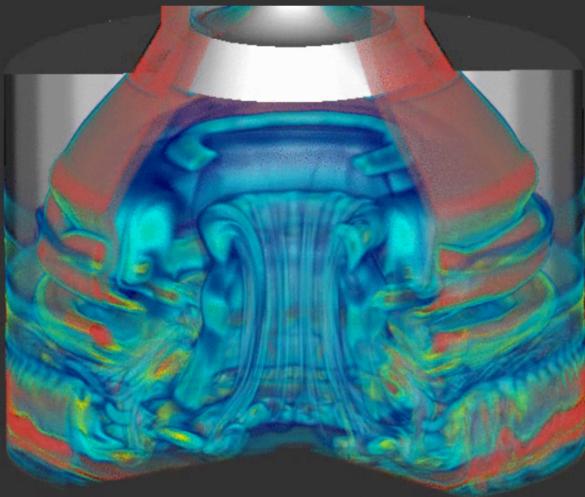


- $Re_c = 400,000$ with 5° angle of attack.
- 3.2 billion gridpoints
- Locally structured data
 - (within each high-order element)
- Globally unstructured mesh

Hosseini, S. M., Vinuesa, R., Schlatter, P., Hanifi, A. and Henningson, D. S.: Direct numerical simulation of the flow around a wing section at moderate Reynolds numbers. In 15th European Turbulence Conference, 25-28 August, 2015, Delft, The Netherlands.

DNS For I.C. Engine Analysis *M. Schmitt, ETH Zurich, 2014*

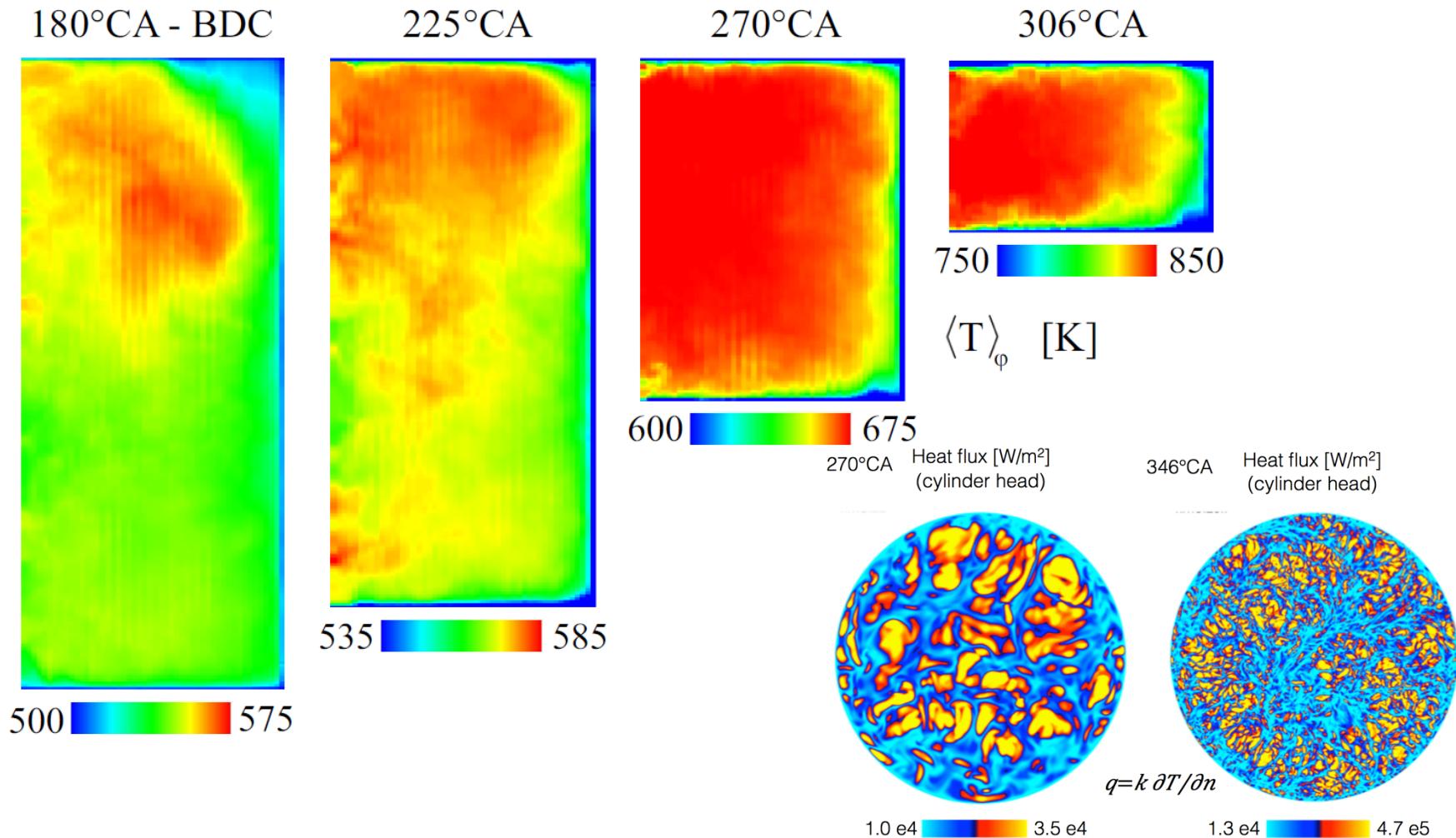
Goals: - cycle-to-cycle var.
- thermal analysis



Compression: Significant Increase in Range of Scales at TDC

— M. Schmitt, ETHZ 2014

Impacts thermal boundary layer, initial conditions for ignition.

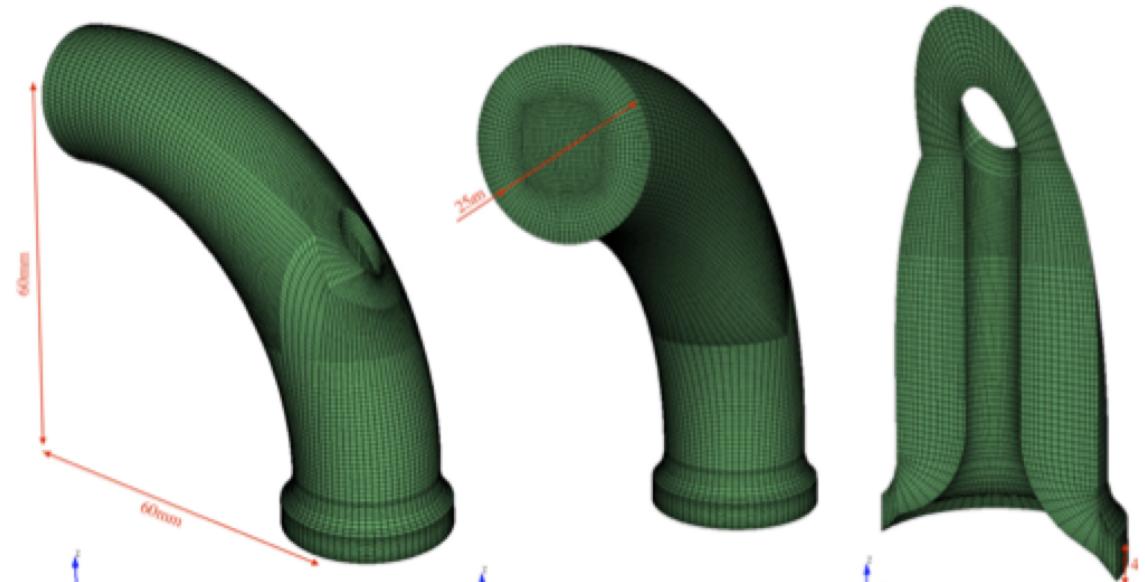
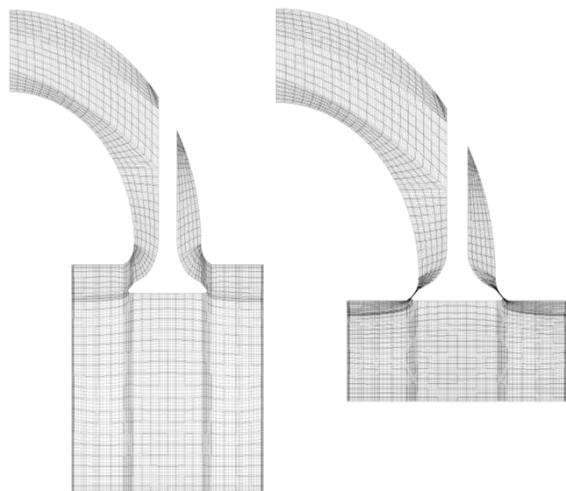
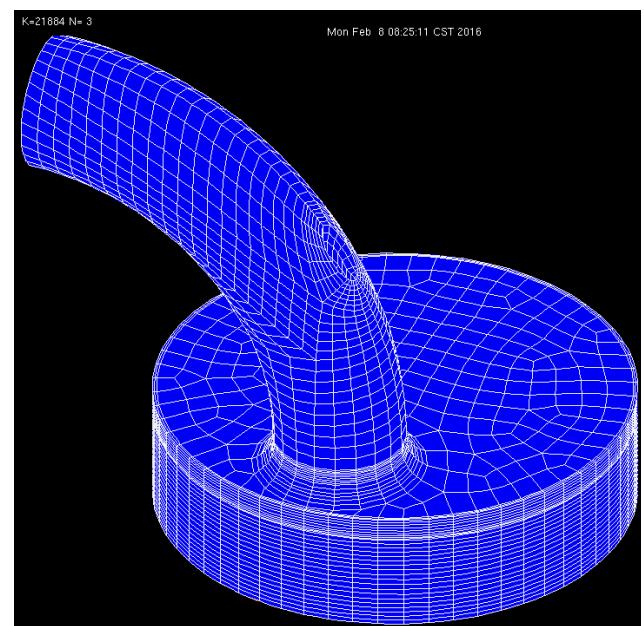
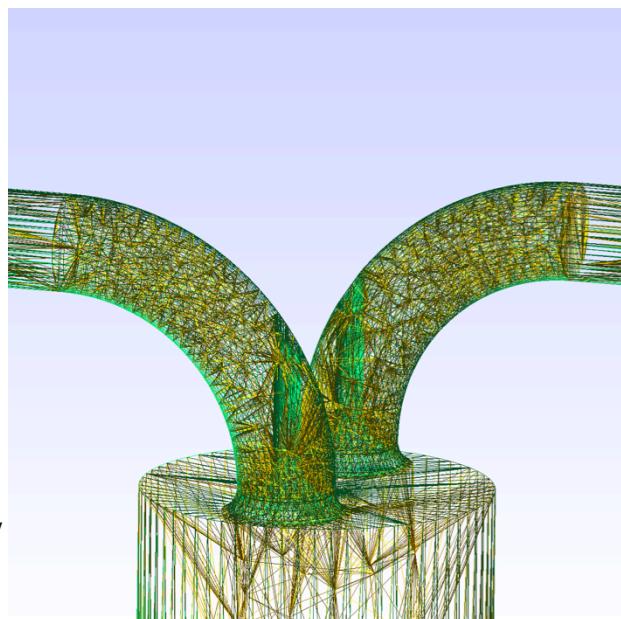


DNS of Turbulence in the TCC Model

Starting with an .stl file,
mesh is made with
CUBIT.

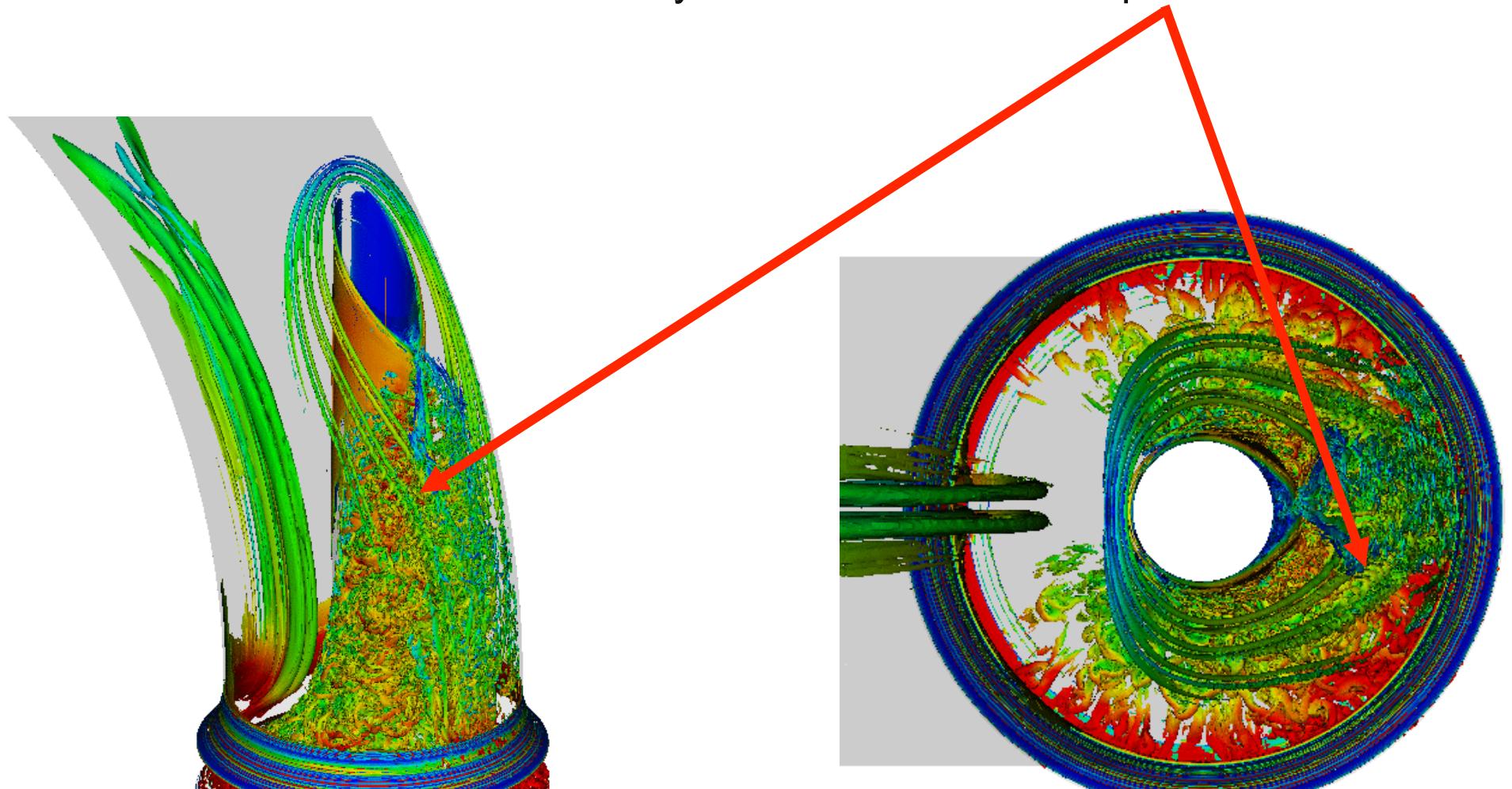
The lower panel shows
the mesh motion.

Lower-right shows a very
fine mesh used for the
intake port.



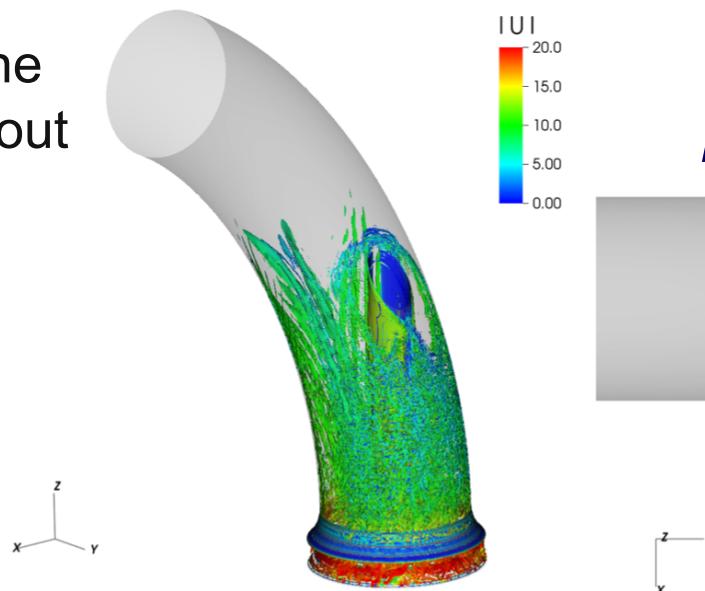
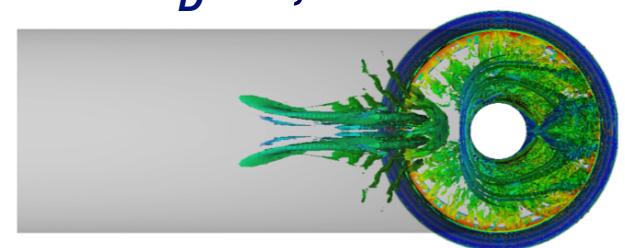
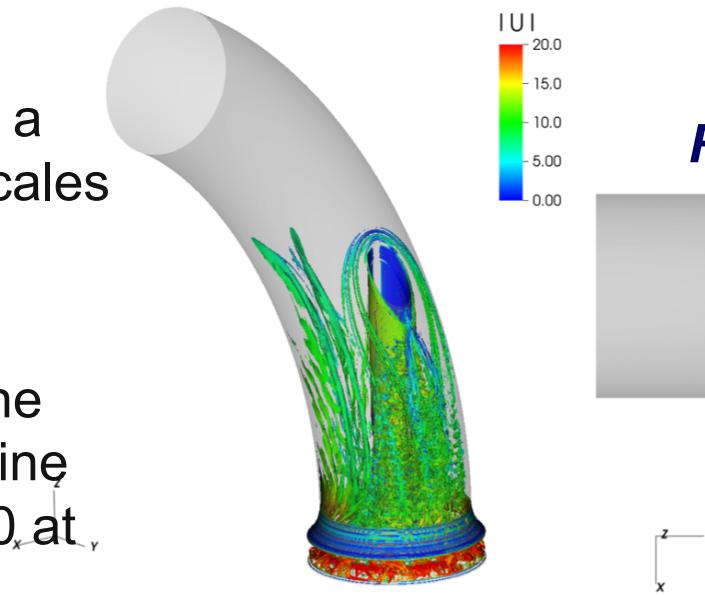
Vortex Breakdown at $Re_D = 15,000$

- These are extremely well resolved calculations performed on Mira.
- Note the highly-resolved filamental horseshoe vortices around the base of the valve stem that ultimately break down into a hairpin vortex chain.



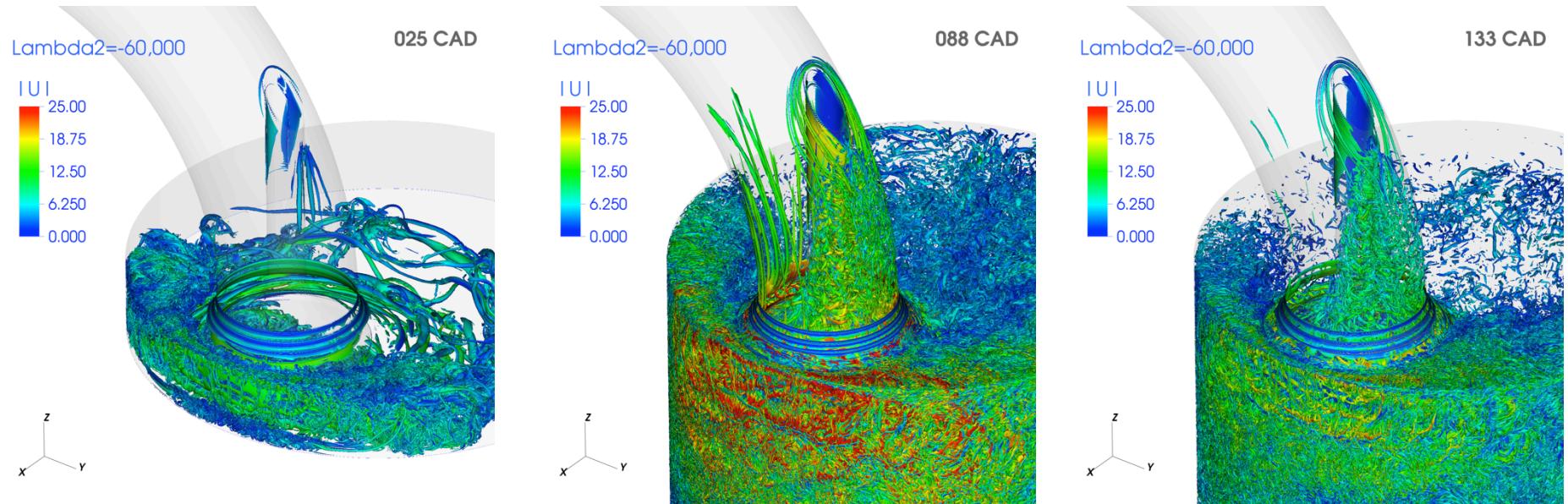
Influence of Reynolds Number

- The Reynolds number has a significant impact on the scales of motion.
- The Reynolds number in the intake port of the TCC engine peaks at around $Re=45000$ at 670 RPM.
- The Reynolds number in the combustion chamber is about $Re=15000$.



Progression in CA

G. Giannakopoulos, ETHZ

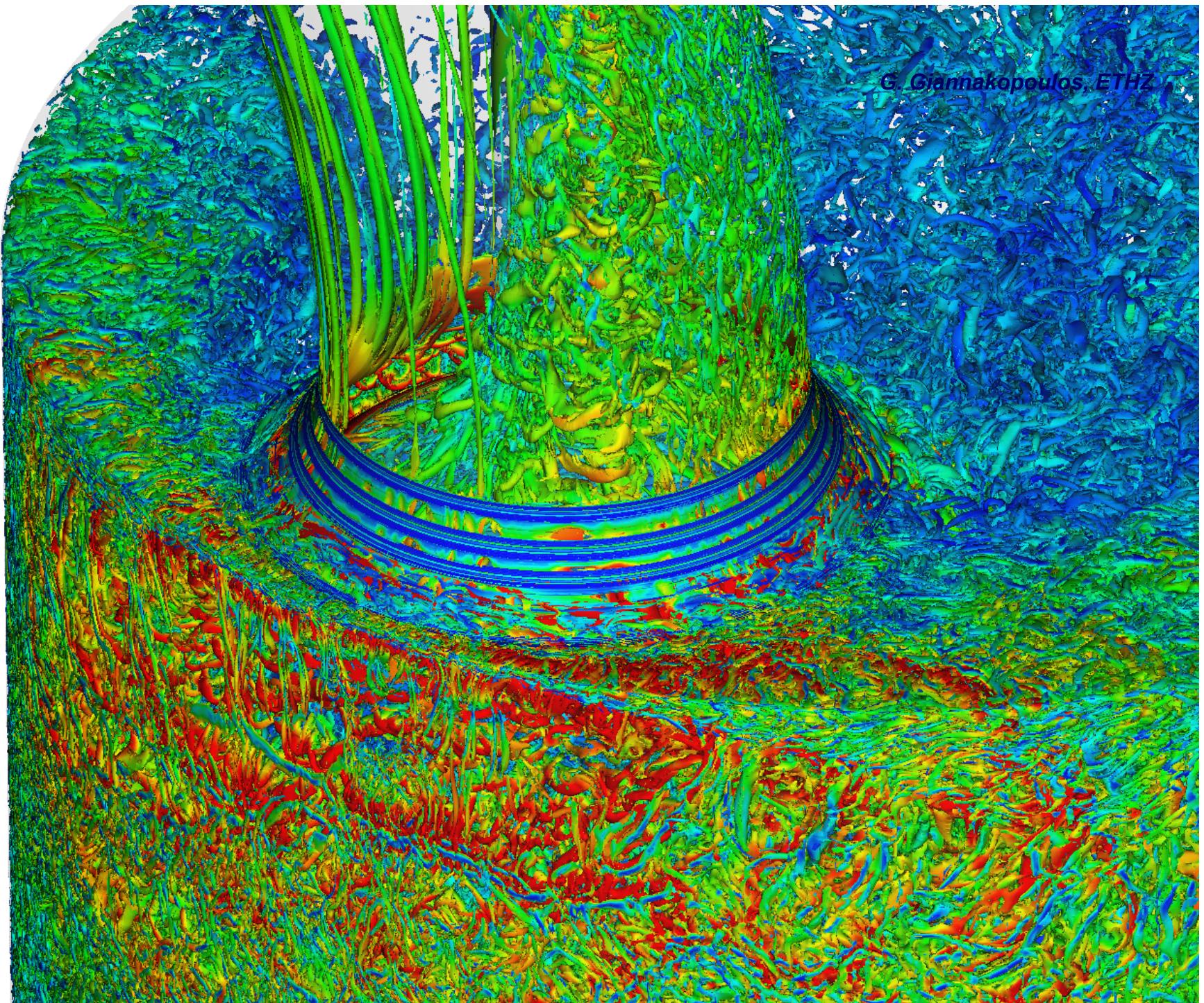


- λ_2 criterion (Jeong & Hussein '95) involves velocity gradients.

$$\lambda_2(\mathbf{S}^2 + \boldsymbol{\Omega}^2) < 0, \quad \mathbf{S} := \frac{1}{2} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T], \quad \boldsymbol{\Omega} := \frac{1}{2} [\nabla \mathbf{u} - (\nabla \mathbf{u})^T]$$

- Places stringent demands on resolution since velocity is only C^0

G. Giannakopoulos, ETHZ

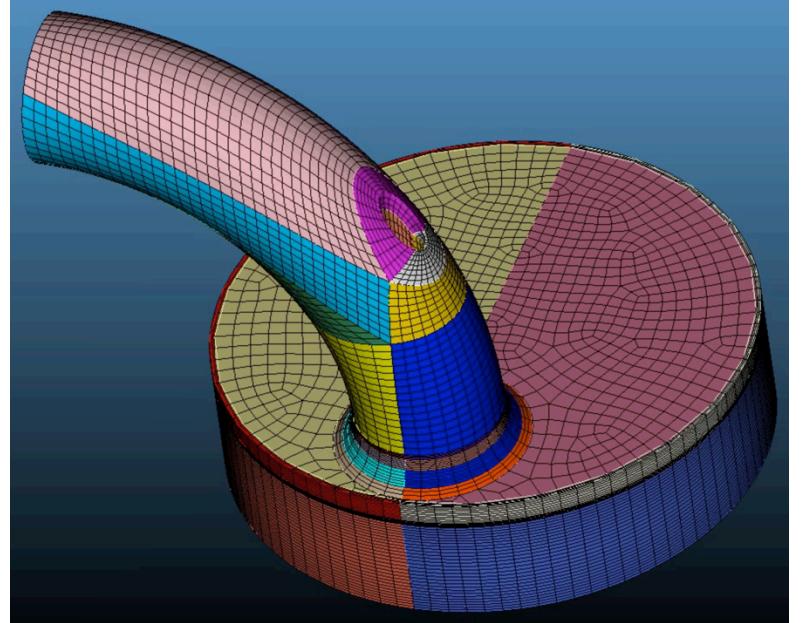


Direct Numerical Simulation Costs

G. Giannakopoulos, ETHZ

- Several meshes, but largest is 3.9 million elements of order N=6:

- $216 \times 3.9 \text{ million} = 840 \text{ million points}$
- 0-180 CAD at 400 RPM
- 100 hours on 131072 cores ($\sim 1/6$ Mira)



- Can we run faster?
 - Better algorithms?
 - *Lower n (via high-order discretizations)*
 - *Faster solvers (lower iteration counts)*
 - More parallelism?

Some Relatively Deep Considerations

- High-Order:
 - reduction in problem size and, hopefully, costs.
- Fast multilevel solvers:
 - coarse-grid solve is a big challenge in parallel
- More parallelism
 - How much more?

Influence of Scaling on Discretization

Large problem sizes enabled by peta- and exascale computers allow propagation of small features (size λ) over distances $L \gg l$. If speed ~ 1 , then $t_{final} \sim L / \lambda$.

- Dispersion errors accumulate linearly with time:

$$\sim |correct\ speed - numerical\ speed| * t \quad (for\ each\ wavenumber)$$

$$\rightarrow error_{t_final} \sim (L / \lambda) * |numerical\ dispersion\ error|$$

- For fixed final error ε_f , require: numerical dispersion error $\sim (\lambda / L) \varepsilon_f \ll 1$.

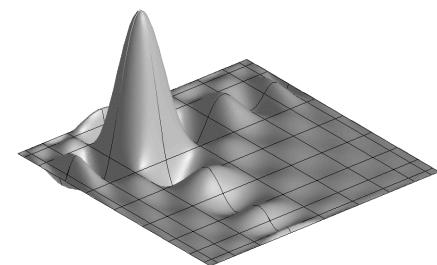
High-order methods can efficiently deliver small dispersion errors.

(Kreiss & Oliger 72, Gottlieb et al. 2007)

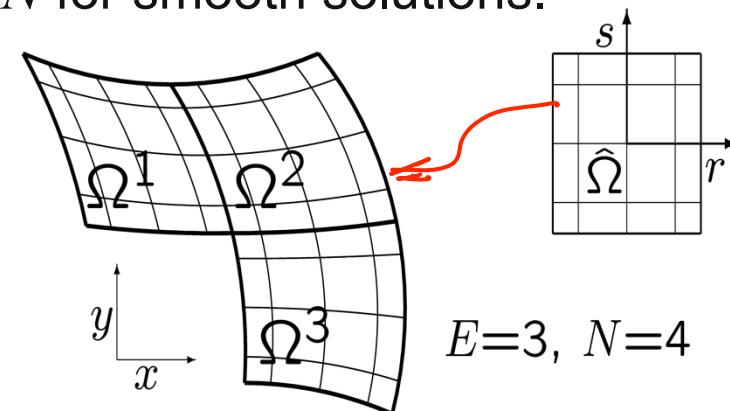
High-Order Spatial Discretizations

Example: Spectral element method (*Patera 84, Maday & Patera 89*)

- Variational method, similar to FEM, using *GL* quadrature.
- Domain partitioned into E high-order hexahedral elements
- Trial and test functions represented as N th-order tensor-product polynomials within each element. ($N \sim 4 \text{--} 15$, typ.)
 - $n \sim EN^3$ gridpoints in 3D
 - Fast operator evaluation: $O(n)$ storage, $O(nN)$ work
- Converges *exponentially fast* with N for smooth solutions.



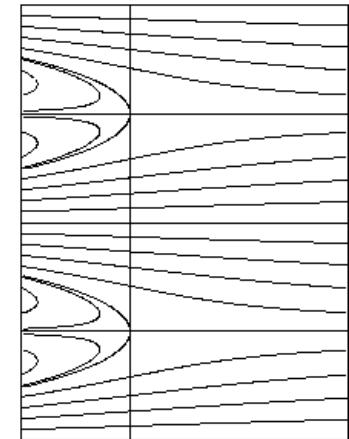
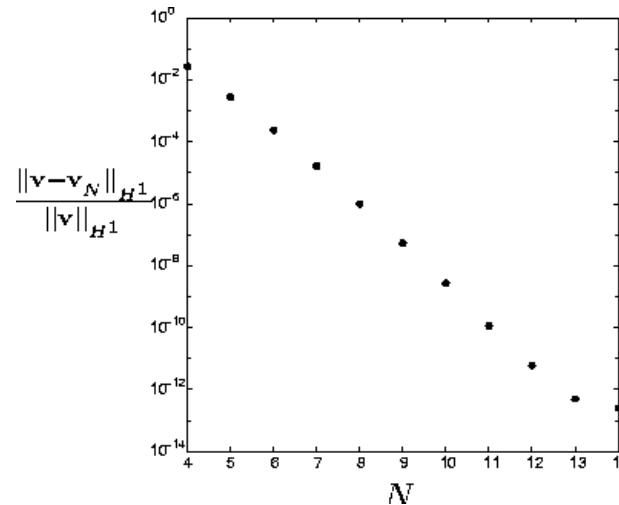
2D basis function, $N=10$



Spectral Element Convergence: Exponential with N

- ❑ 4 orders-of-magnitude error reduction when doubling the resolution in each direction

Exact Navier-Stokes Solution (Kovazsnay '48)



- ❑ For a given error,

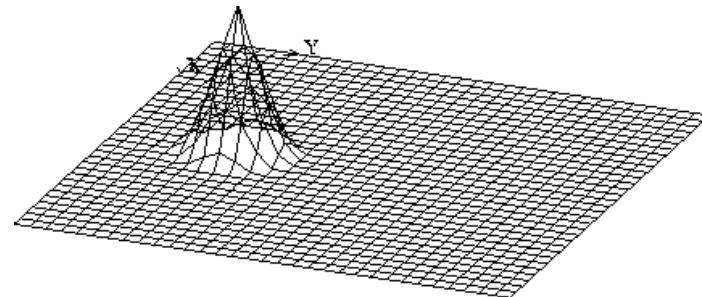
- ❑ Reduced number of gridpoints
- ❑ Reduced memory footprint.
- ❑ Reduced data movement.

$$v_x = 1 - e^{\lambda x} \cos 2\pi y$$

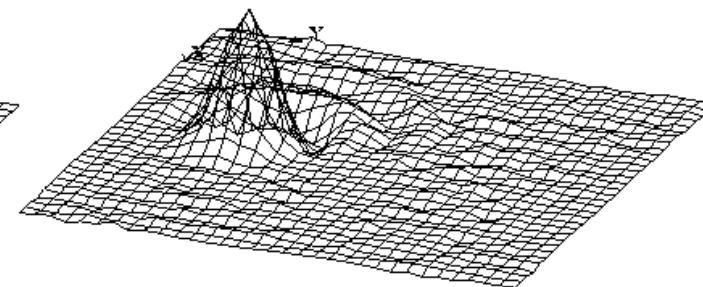
$$v_y = \frac{\lambda}{2\pi} e^{\lambda x} \sin 2\pi y$$

$$\lambda := \frac{Re}{2} - \sqrt{\frac{Re^2}{4} + 4\pi^2}$$

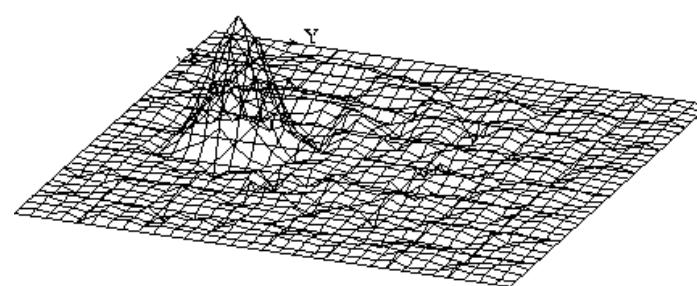
Excellent transport properties, even for non-smooth solutions



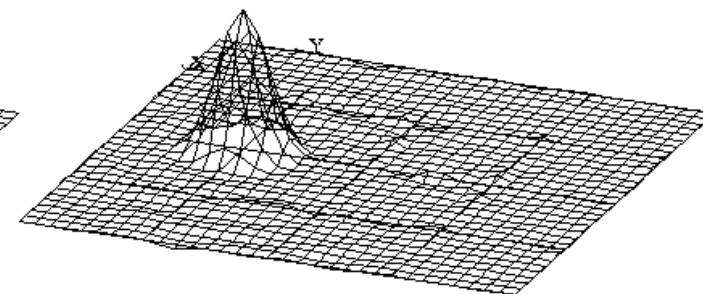
Initial Condition



$K_1 = 16, N = 2$



$K_1 = 8, N = 4$



$K_1 = 4, N = 8$

Convection of non-smooth data on a 32x32 grid.

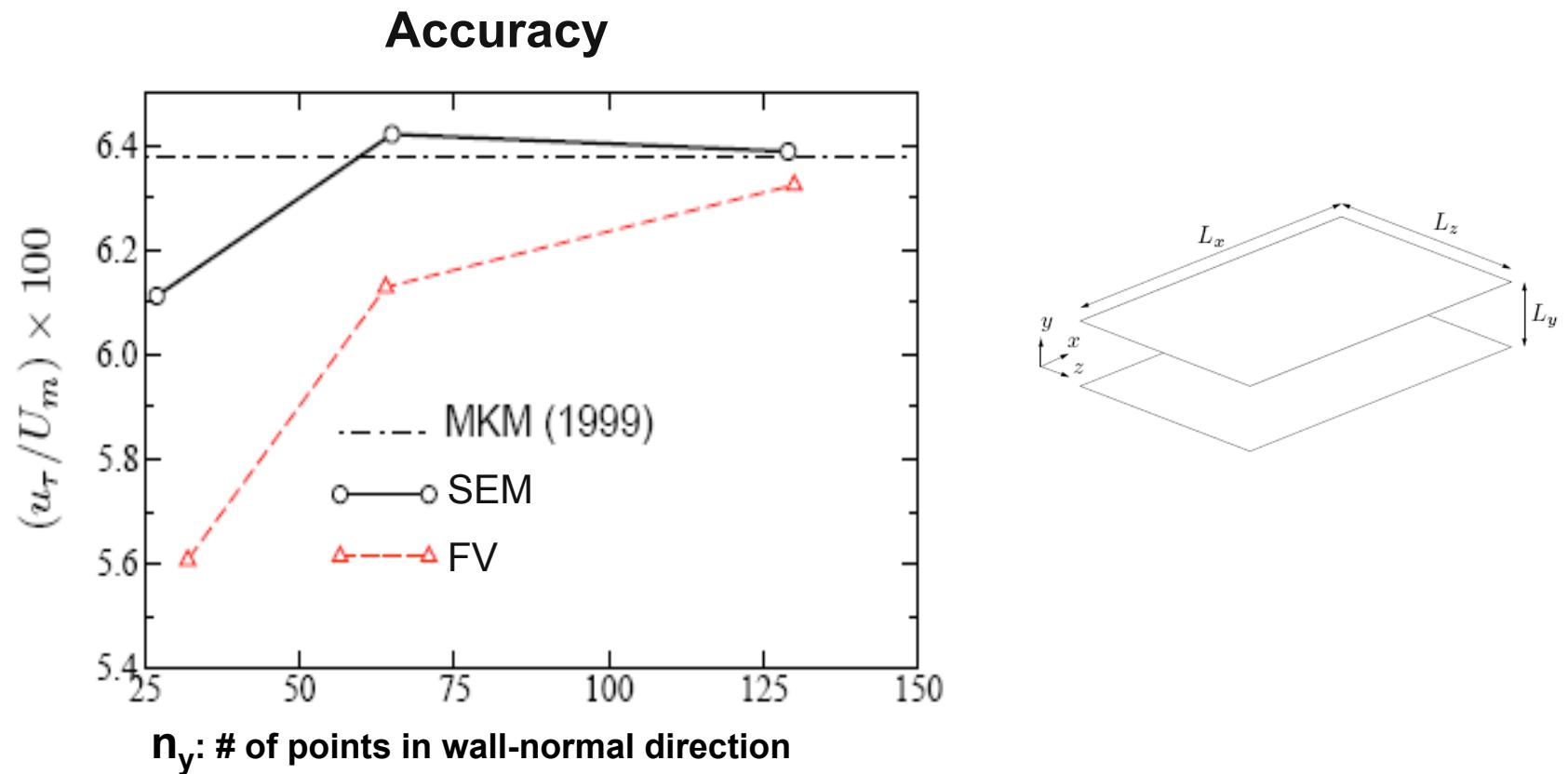
($K_1 \times K_1$ spectral elements of order N).

(cf. Gottlieb & Orszag 77)

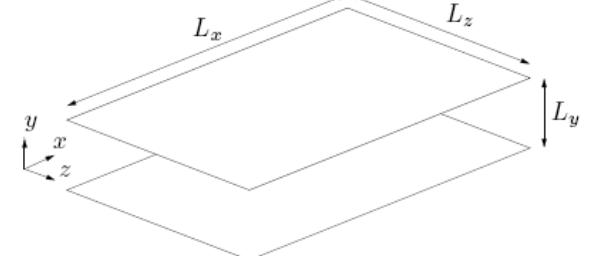
Nonlinear Example: NREL Channel Flow Study

Sprague et al., 2010

- **Accuracy:** Comparison to several metrics in turbulent DNS, $\text{Re}_\tau = 180$ (MKM' 99)



- 7th-order SEM needs an *order-of-magnitude* fewer points than 2nd-order FV.

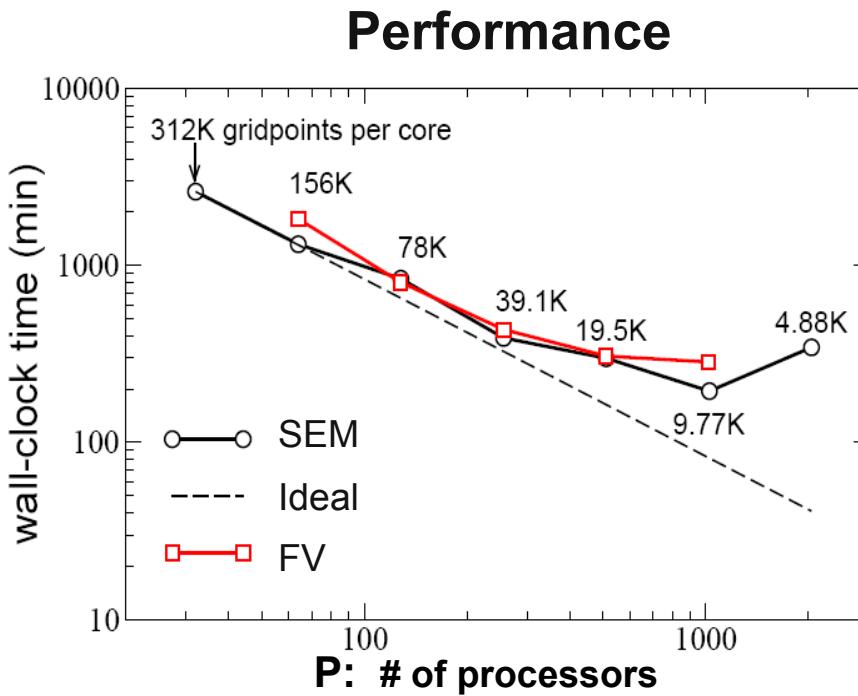
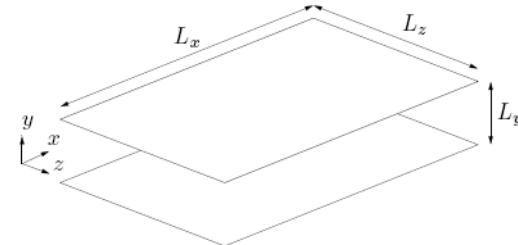


Nonlinear Example: NREL Channel Flow Study

Sprague et al., 2010

Benefits in linear
problems carry over to
nonlinear case.

- Test case: DNS $Re_t = 180$ (MKM' 99)



- Results: — Properly implemented SEM and FV have the *same* cost per gridpoint

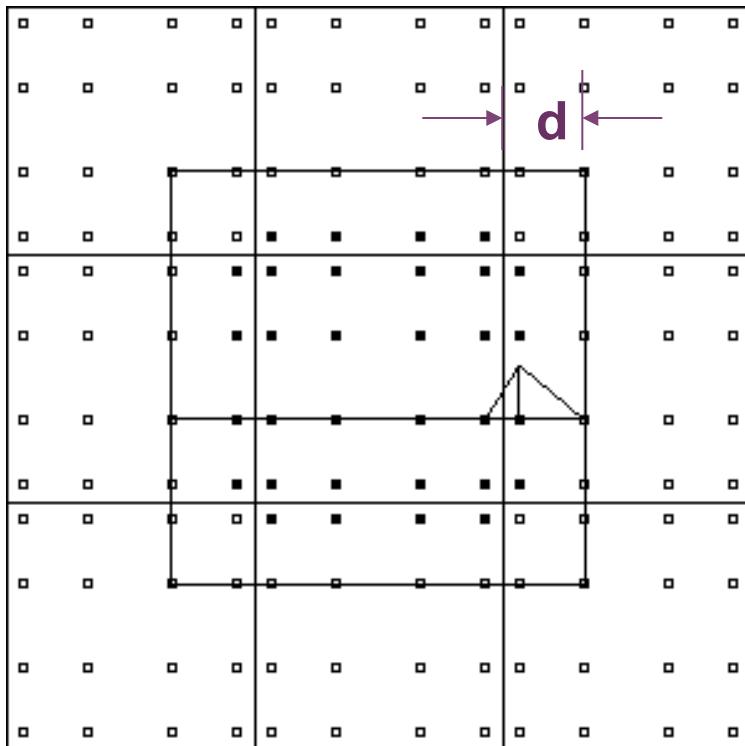
Some Relatively Deep Considerations

- High-Order:
 - reduction in problem size and, hopefully, costs.
- Fast multilevel solvers:
 - coarse-grid solve is a big challenge in parallel
- More parallelism
 - How much more?

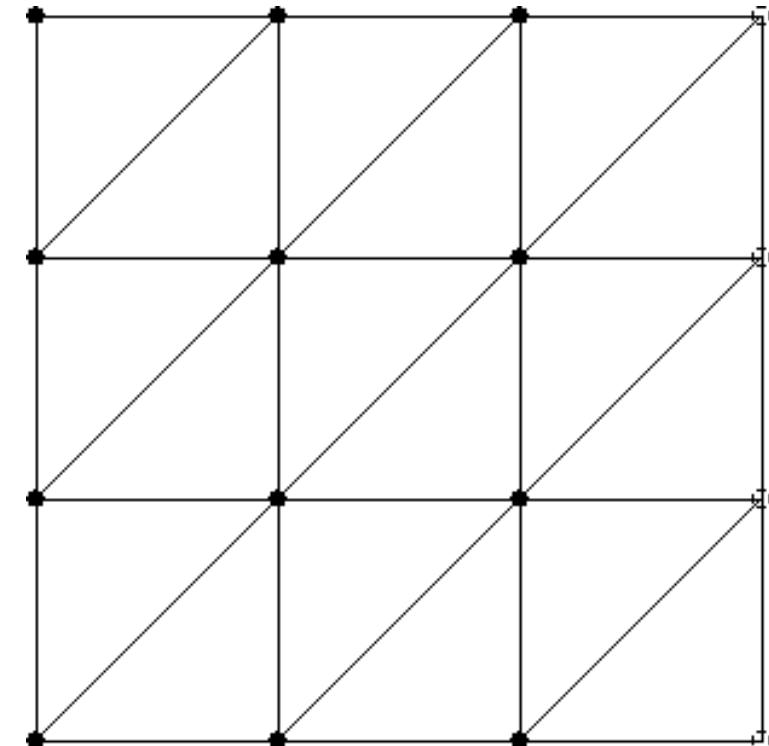
Fast Multilevel Solvers

Multigrid with Additive Schwarz-Based Smoothing

$$\underline{z} = M\underline{r} = \sum_{e=1}^E R_e^T A_e^{-1} R_e \underline{r} + R_0^T A_0^{-1} R_0 \underline{r}$$



Local Overlapping Smoother: FEM-based
Poisson problems with homogeneous
Dirichlet boundary conditions, A_e .
Use fast diagonalization.



Coarse Grid Solve: Poisson problem
using linear finite elements on entire
spectral element mesh, A_0 (**GLOBAL**).

(Dryja & Widlund 87, Pahl 93, Lottes & F 05)

Fast Solvers for p -Multigrid

- Schwarz Smoothers: fast diagonalization method (*Rice et al. 64, Couzy 95, F.02*)

- **Exploit local tensor-product structure:**

$$A_e^{-1} = (S \otimes S) (I \otimes \Lambda_x + \Lambda_y \otimes I)^{-1} (S \otimes S)^T$$

- Complexity $< A p$

- p -multigrid schedule:

$$N_f = N$$

$$N_1 = 3$$

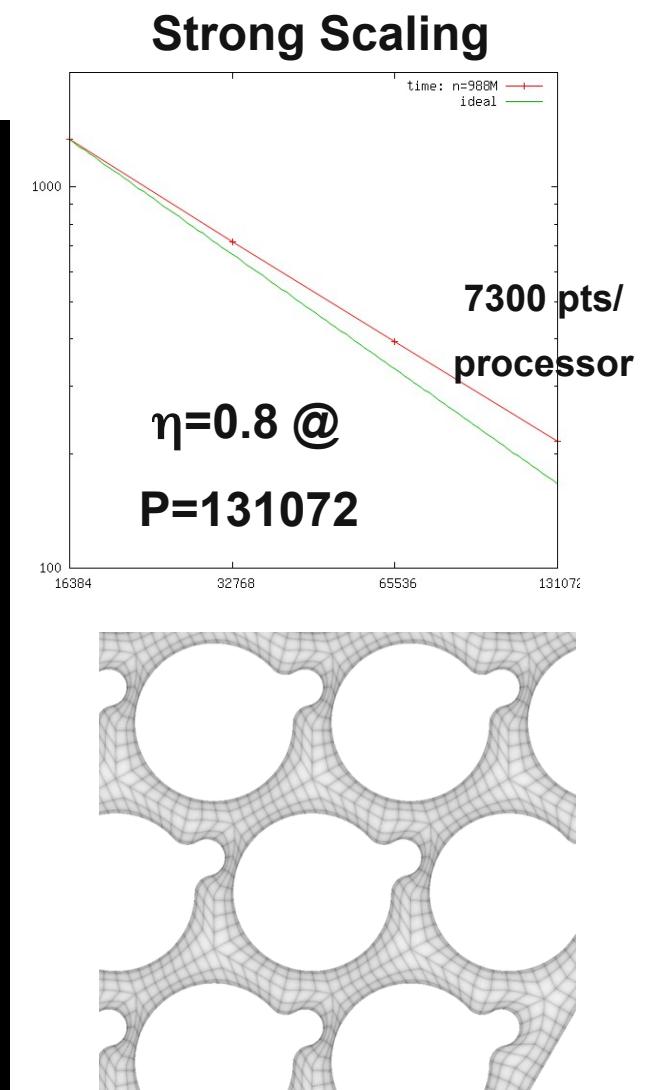
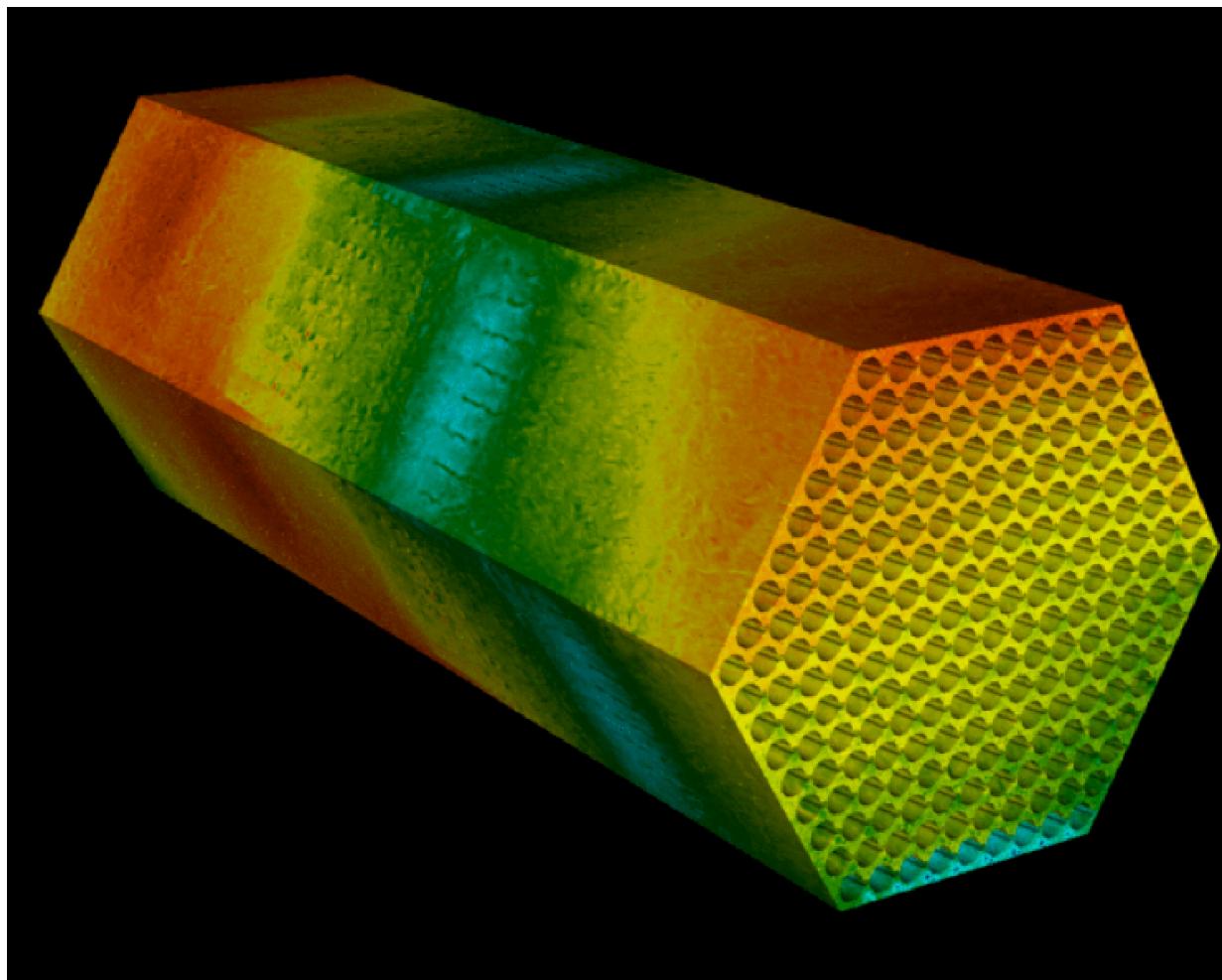
$N_0 = 1$ (coarse-grid solve)

- **Coarse-grid solve:** Direct, XX^T (F. & Tufo 01) – $P \sim 100,000$ or less
Custom AMG: (Lottes 08/11) – $P \sim 10^5 \dots 10^9$

Communication intensive!

Putting At All Together: Subassembly with 217 Wire-Wrapped Pins

- 3 million 7th-order spectral elements (n=1.01 billion)
- 16384–131072 processors of IBM BG/P
- 15 iterations per timestep; 1 sec/step @ P=131072
- Coarse grid solve < 10% run time at P=131072



More Parallelism?

More Parallelism?

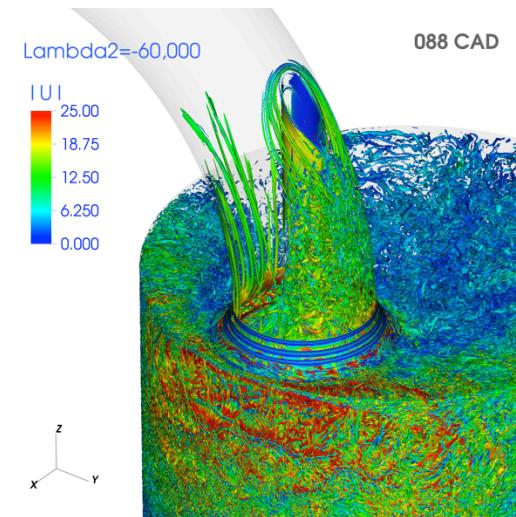
- Current simulation has 3.9 million elements.

- Therefore, max value of P is 3.9 M.
 - $\rightarrow n/P \sim 216$ points per processor.
 - **Too Low.**

- Why?

- Back of the envelope analysis suggests a minimum of $n/P \sim 2000$ points per MPI rank on Mira to realize 50% parallel efficiency
 - **for any finite difference/volume/element code.**(Based on communication cost overhead, rate of local work, etc.)

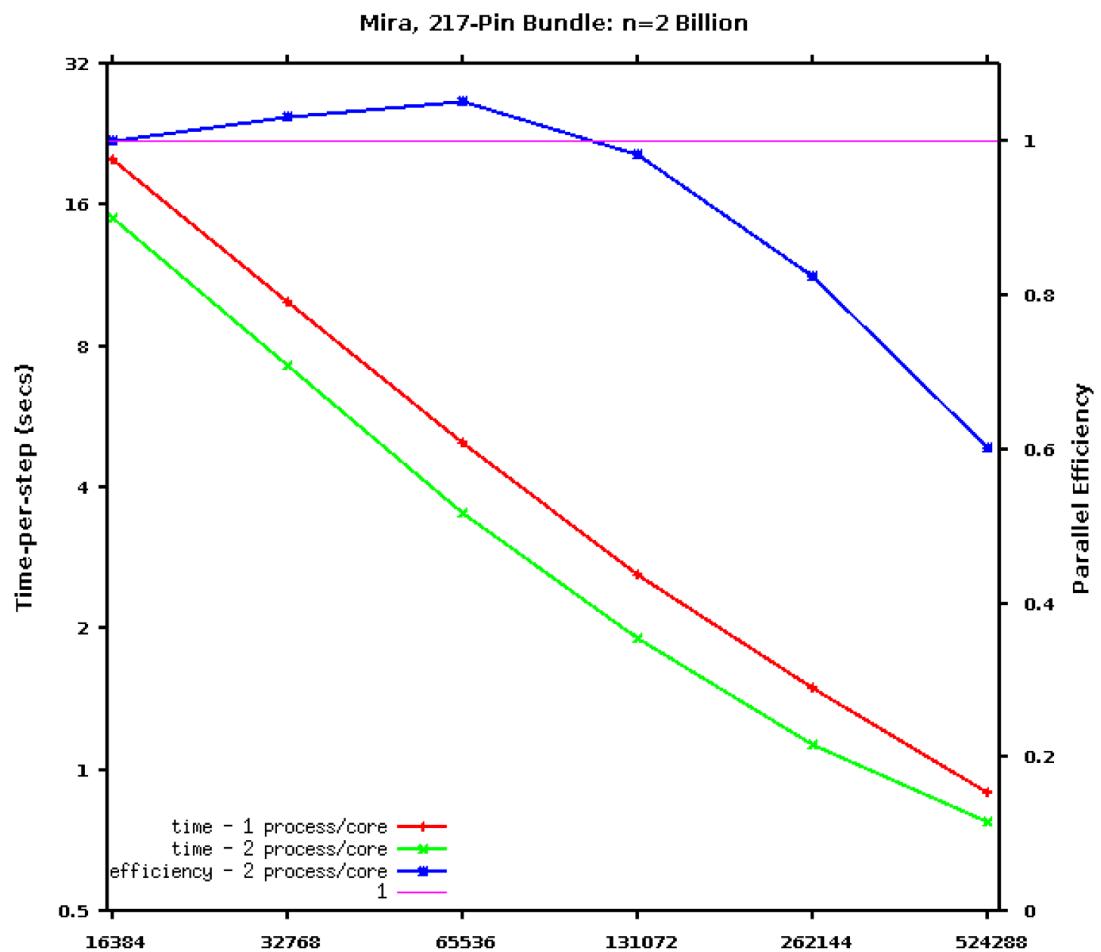
- Current simulations are at $n/p \sim 8.4M/262144 \sim 3200$.



Scaling to Beyond 1 Million Processes

217 Pin Problem, N=9, E=3e6:

- 2 billion points
- BGQ – 524288 cores
 - 1 or 2 ranks per core
- A mixture of CG / multigrid
- 60% parallel efficiency at 1 million ranks
- *2000 points/rank at 1 million ranks*



Scaling Questions

- Will this scaling continue?
- Is this the best we can do?
- What, exactly, is better, or even good?
 - Good node performance
 - **Strong** scaling to large processor counts.
- Strong scaling is ultimately limited by costs that do not go to zero as $n/P \rightarrow 0$:

$$t \sim c_1 n/P + c_2 + c_3 \log P$$

- c_2 ~ communication overhead
 - ~ other overhead (memory latency on GPU)
 - ~ Amdahl
- c_3 ~ can be mitigated by communication hardware

- We are interested in understanding what is setting the limits on strong scaling applications, because that sets the limits on speed.

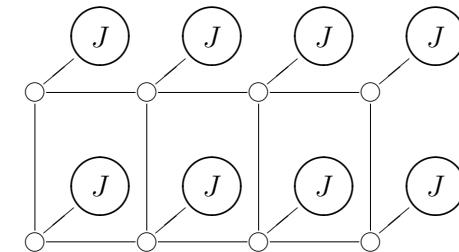
Last Part of Talk

■ Performance Analysis

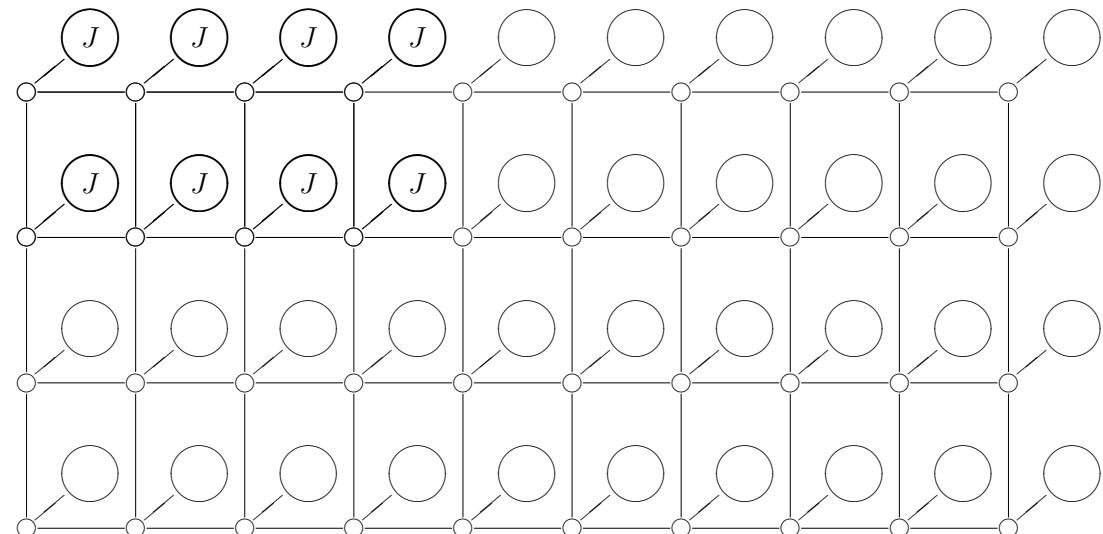
- How can we judge if we're getting any speed up?
 - *Obvious answer is to fix the problem size, and then run on ever larger numbers of processors (or fewer, until you can't fit into memory).*
- Second part is to ask yourself, why I am not seeing more speed-up for the given problem size, n, and number of processors, P ?

Two Run-Time Scenarios

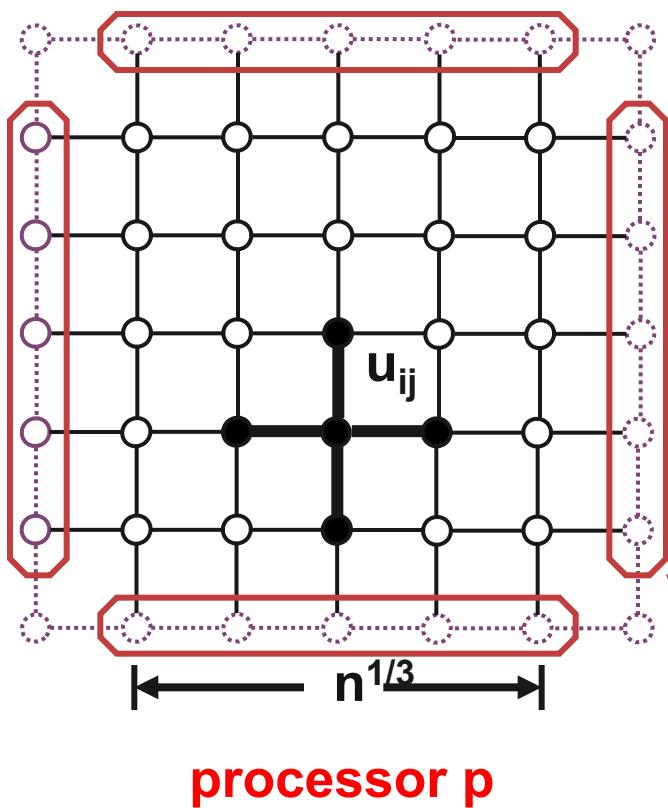
- **Fully Populated Cluster:** job on every node.



- **Supercomputing Center:**
 - Job not using all nodes.
- Our question:
 - *Why stop at P nodes, instead of $2P$??*
- Study model Poisson problem to get insight.
(PDE + HPC)



Model Problem: Poisson with finite differences



- Consider complexity estimates for 3D Poisson with several iterative solvers.
- n/P points on each processor

**data from neighbor
allows stencil update**

Metric for Scalability

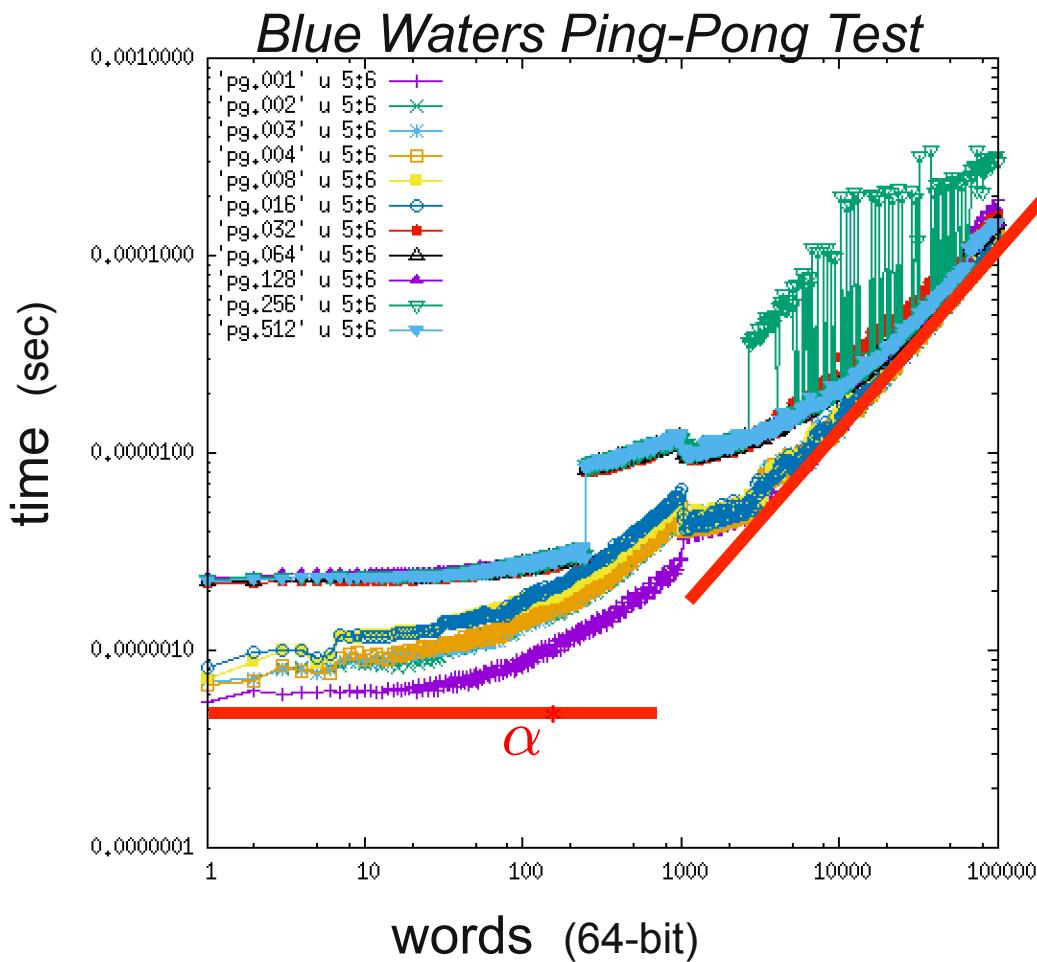
- P-processor solution time for n points:

- $T(P,n) = TA(P,n) + TC(P,n)$, **or** *nonoverlapping comm.*
 - $T(P,n) = \max (TA(P,n) , TC(P,n))$ *overlapping comm.*

- Seek conditions where communication is subdominant, $T_A > T_C$:

- $T_A(P,n) = T(1,n) / P$ the parallel work
 - $T_C(P,n)$ the total communication cost = sum $t_c(m)$

Linear Communication Model



Linear communication model :

$$t_c(m) = \alpha^* + \beta^* m,$$

m = number of 64-bit words

Nondimensionalize by t_a [$c = a^* b$] :

$$t_c(m) = (\alpha + \beta m) t_a$$

$$\alpha = \alpha^* / t_a, \quad \beta = \beta^* / t_a$$

Linear Communication Model

- Simple (simplistic?) and general:
 - Determined by two asymptotes (α, β)
 - Does not capture contention effects.
 - Are these *important? Probably, on rich nodes.*
 - Our approach: model *ideal* performance and investigate departures from ideal.
- More complex models depend on
 - P
 - Runtime topology – rarely known (except on Bluegene)
 - Other jobs in system (except on Bluegene)
 - Node architecture
 - (e.g., Gropp, Olson, Samfass 2016: *Modeling MPI Communication Performance on SMP Nodes: Is it Time to Retire the Ping Pong Test?*)

Modeling MPI Communication Performance on SMP Nodes: Is it Time to Retire the Ping Pong Test?

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ABSTRACT

The “postal” model of communication [3, 8] $T = \alpha + \beta n$, for sending n bytes of data between two processes with latency α and bandwidth $1/\beta$, is perhaps the most commonly used communication performance model in parallel computing. This performance model is often used in developing and evaluating parallel algorithms in high-performance computing, and was an effective model when it was first proposed. Consequently, numerous tests of “ping pong” communication have been developed in order to measure these parameters in the model. However, with the advent of multicore nodes connected to a single (or a few) network interfaces, the model has become a poor match to modern hardware

understand performance issues in applications. One of the earliest, sometimes called the postal model [3, 8]², represents the communication time to send n bytes as

$$T = \alpha + \beta n, \quad (1)$$

where the term α denotes the total *latency* and β the inverse of the asymptotic *bandwidth* (for arbitrarily large n , measured in seconds per byte). While numerous other performance models have been proposed [16] and have found some use, the postal model remains the most common performance model used to analyze message-passing programs.

Consequently, many benchmarks measure α and β by sending a message to another process followed by sending the

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Scaling Limits for PDE-Based Simulation

Paul F. Fischer^{*†}

Katherine Heisey[†]

Misun Min[‡]

We analyze algorithm/architecture performance characteristics that have a direct impact on the scalability of present-day and future turbulent flow simulations on large-scale parallel computers.

I. Introduction

Parallel computing is founded on the principle that, given enough work for a given problem, one can subdivide the computation across P processors and realize an effective P -fold reduction in time to solution. On today's architectures, any PDE-based or particle-based simulation that uses a billion gridpoints or particles can easily be distributed across two compute nodes and run in half the time—for essentially the same power—compared with running on just a single node. This computational scenario, running a problem of *fixed size* in half the time on two processors or nearly one- P th the time on P processors, is termed *strong scaling* and is the focus of this paper. Specifically, we explore the basic question of how far one can scale a given problem, defined by its computational resolution n (e.g., the number of gridpoints), when using P processors.

The relevance of the strong scaling question is expressed succinctly in the equation

$$S_P = \eta P S_1, \quad (1)$$

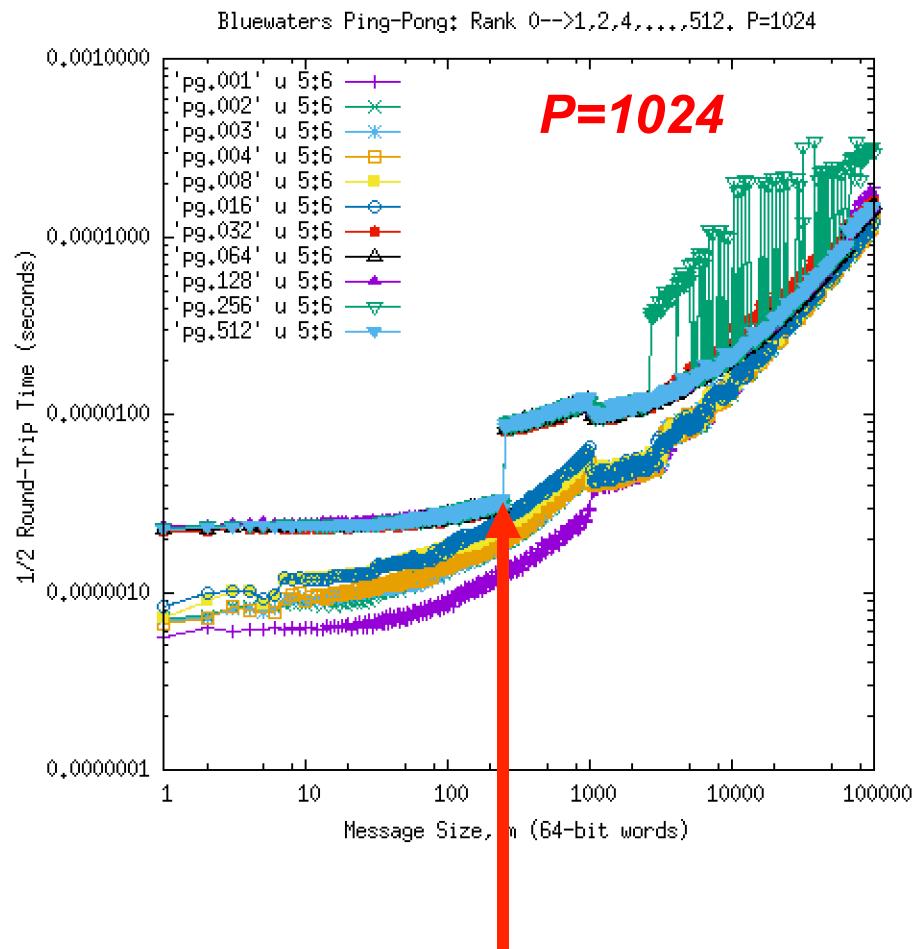
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AIAA 2015

Linear Communication Model

- Simple (simplistic?) and general:
 - Determined by two asymptotes (α, β)
 - Does not capture contention effects.
 - Are these *important? Probably, on rich nodes.*
 - Our approach: model *ideal* performance and investigate departures from ideal.
- More complex models depend on
 - P
 - Runtime topology – rarely known (except on Bluegene)
 - Other jobs in system (except on Bluegene)
 - Node architecture
 - (e.g., Gropp, Olson, Samfass 2016: *Modeling MPI Communication Performance on SMP Nodes: Is it Time to Retire the Ping Pong Test?*)

Linear Communication Model – P dependence

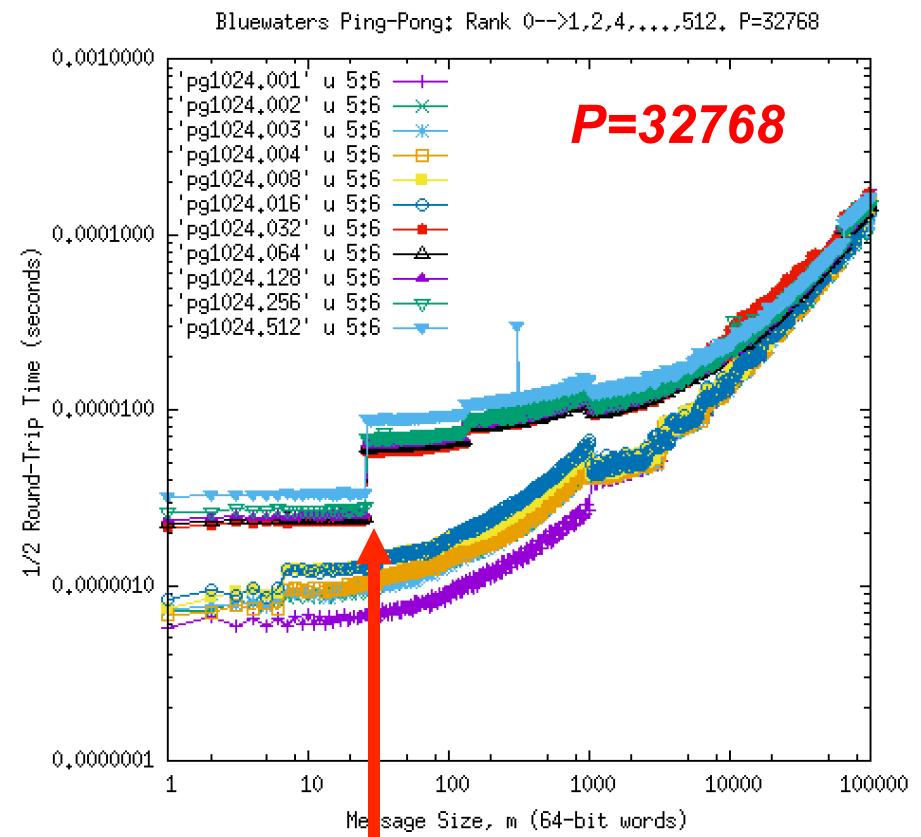
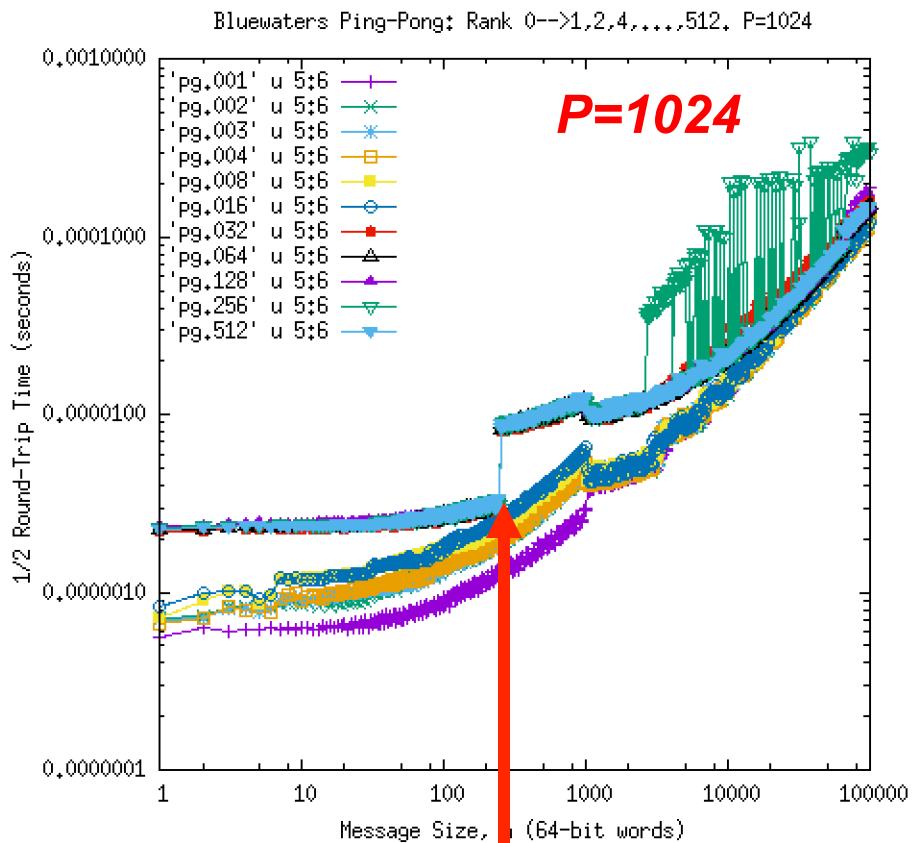


- Switch to 3-trip messaging:
 - Source: “ n bytes coming, ready?”
 - Target: “ready”
 - Source: n bytes → target

Linear Communication Model – P dependence

- The switch point is important in the strong-scale limit $n/P \rightarrow 0$
 - Communication costs are significant (surface/volume large)
 - Messages are short:
 - $m < m_{switch}$: $Cost \sim \alpha$
 - $m > m_{switch}$: $Cost \sim 3\alpha$
- Switch point is reduced when P increases
 - Need to reserve P buffers of size b : local memory demand scales as $(P \times b)$
 - Inveighs against strong scaling.
- For PDEs, we don't need a lot of large buffers.
 - Rare is the 3D application where ranks talk actively to more than 100 other ranks.
 - **We should boost buffer sizes on most active rank-to-rank exchanges.**
 - **Reduce (eliminate) unused set-aside buffers.**
 - Maybe already in place? (A question to MPI experts in the audience..)

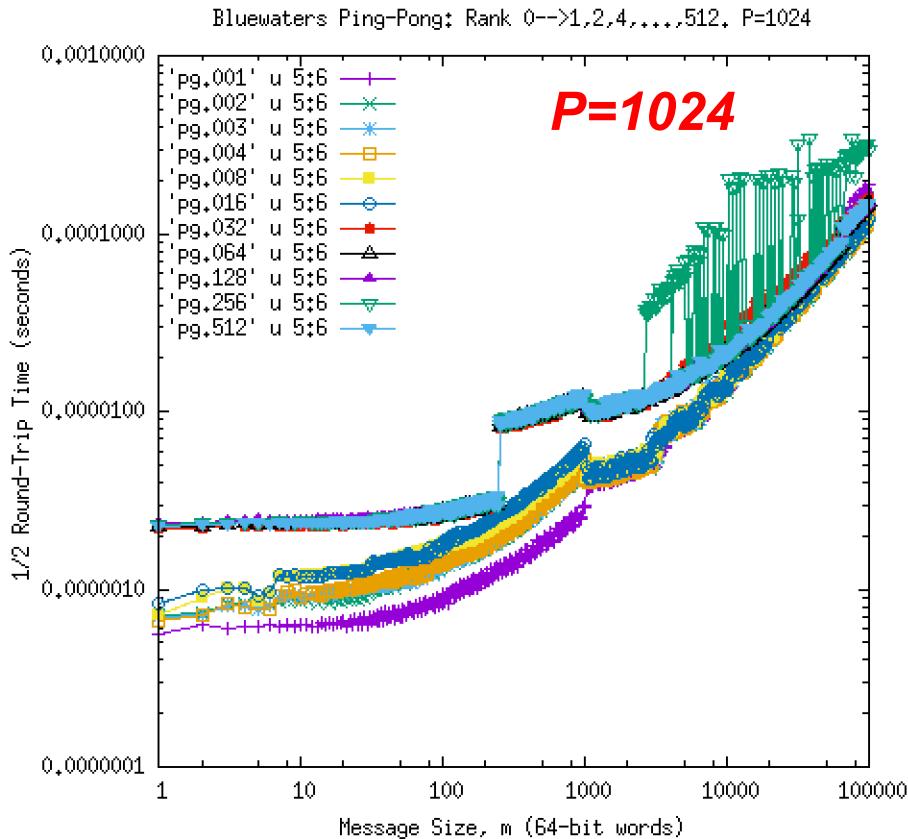
Linear Communication Model – P dependence



- Switch to 3-trip messaging:
 - Source: “n bytes coming, ready?”
 - Target: “ready”
 - Source: n bytes → target

- Larger $P \rightarrow$ smaller buffers
 - “Short messages” are shorter

Linear Communication Model – P dependence

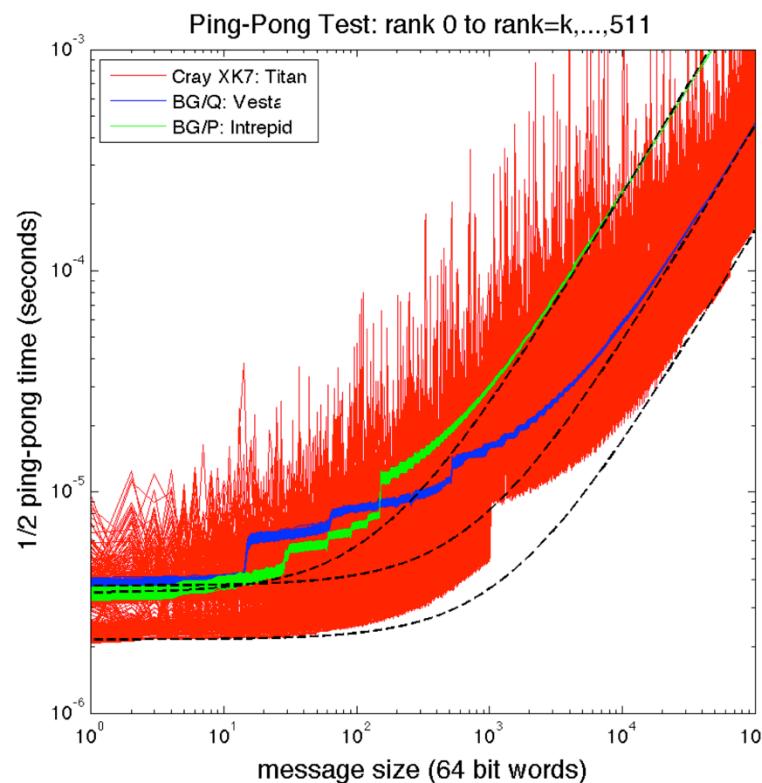


Target	P	nloop	m	time	time/wd
512	1024	84	239	3.30592905E-06	1.38323391E-08 pg
512	1024	82	242	3.36620866E-06	1.38527105E-08 pg
512	1024	81	247	2.95962816E-06	1.19823003E-08 pg
512	1024	80	251	8.53762031E-06	3.40144235E-08 pg
512	1024	78	256	9.70474175E-06	3.43544600E-08 pg
512	1024	77	261	8.73401568E-06	3.34636616E-08 pg
512	32768	668	23	3.32483274E-06	1.44557945E-07 pg
512	32768	642	24	3.36060643E-06	1.40025268E-07 pg
512	32768	618	25	3.36042886E-06	1.34417154E-07 pg
512	32768	596	26	8.83548852E-06	3.39826481E-07 pg
512	32768	576	27	8.77430042E-06	3.24974089E-07 pg
512	32768	557	28	8.73384613E-06	3.11923076E-07 pg

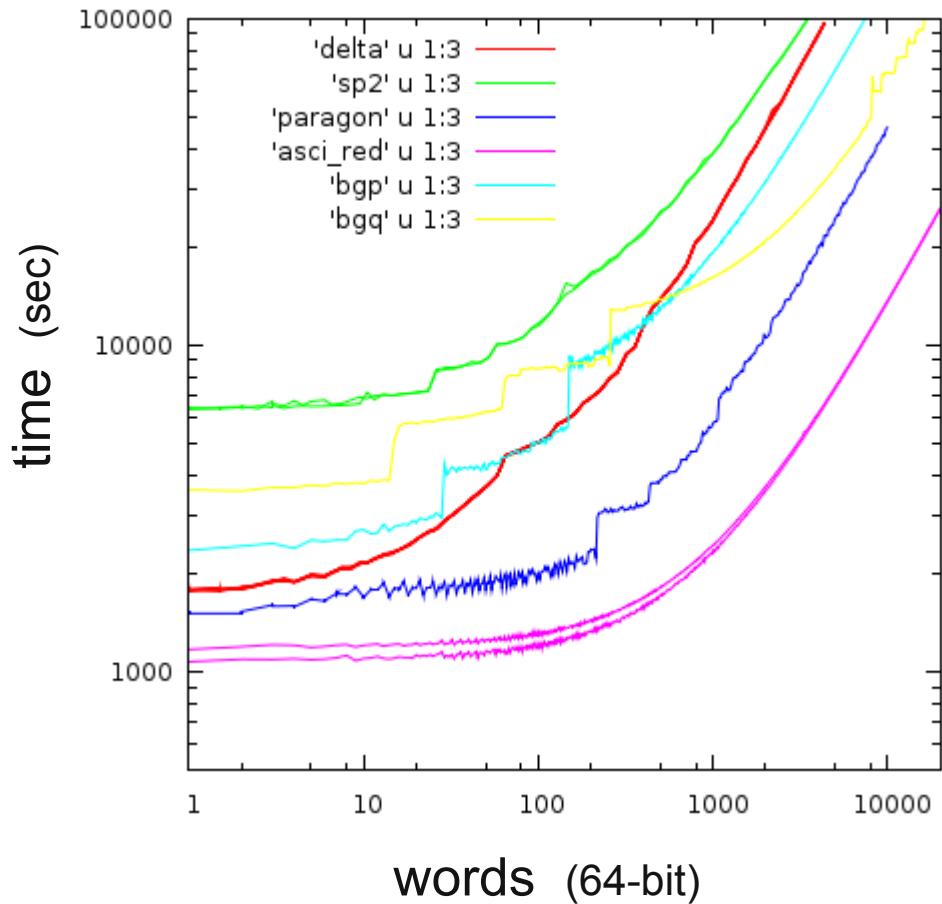
- Going from P=1024 to P=32768 on BW
 - Switchpoint between short and long messages moves from 250 words to 25 words.
- If you have $10^3 = 1000$ points/rank, need switchpoint to be $\sim 100 = 10^2$

Linear Communication Model – P dependence

- Another argument for (or against) the simple linear communication model...
- System noise is difficult to quantify



Linear Communication Model over Several Decades Nondimensionalized!



Linear communication model :

$$t_c(m) = \alpha^* + \beta^* m, \quad m: 64\text{-bit words}$$

Nondimensionalize by t_a [c = a*b] :

$$t_c(m) = (\alpha + \beta m) t_a$$

$$\alpha = \alpha^* / t_a, \quad \beta = \beta^* / t_a$$

30 Years of Nondimensional Machine Parameters

Year	t_a (μ s)	αt_a (μ s)	βt_a (μ s/wd)	α	β	m_2	machine
1986	50	5960	64	119.2	1.28	93	Intel iPSC-1 (286)
1987	0.333	5960	64	17898	192	93	Intel iPSC-1/VX
1988	10	938	2.8	93.8	0.28	335	Intel iPSC-2 (386)
1989	0.25	938	2.8	3752	11.2	335	Intel iPSC-2/VX
1990	0.1	80	2.8	800	28	29	Intel iPSC-i860
1991	0.1	60	0.8	600	8	75	Intel Delta
1992	0.066	50	0.15	760	2.3	333	Intel Paragon
1995	0.02	60	0.27	3000	13.5	222	IBM SP2 (BU96)
1996	0.016	30	0.02	1875	1.25	1500	ASCI Red 333
1998	0.006	14	0.06	2333	10	233	SGI Origin 2000
1999	0.005	20	0.04	4000	8	500	Cray T3E/450
2005	0.002	4	0.026	2000	13	154	BGL/ANL
2008	0.0017	3.5	0.022	2060	13	160	BGP/ANL
2011	0.0007	2.5	0.002	3570	2.87	1250	Cray Xe6 (KTH)
2012	0.0007	3.8	0.0045	5430	6.43	845	BGQ/ANL
2015	0.0004	2.2	0.0015	5500	3.75	1467	Cray XK7

- $m_2 := \alpha / \beta \sim$ message size \rightarrow twice cost of single-word message
- t_a based on noncached matrix-matrix products of order 10—13

Scalability Estimates: Jacobi Iteration

Point Jacobi iteration (7-point stencil):
$$u_i = \frac{1}{a_{ii}}(f_i - \sum_{j \neq i} a_{ij}u_j)$$

- Work: $T_{aJ} \sim 14 n/P t_a$
- Communication: $T_{cJ} \sim (6 + (n/P)^{2/3} (1/m_2)) \alpha t_a$
- For fixed n/P , Jacobi complexity is P-independent
.assuming P independent message costs; no contention.
- However, algorithmic scaling is poor (iteration count scales as $n^{2/3}$)
 - a more communication intensive approach is required
 - conjugate gradient iteration, multigrid, etc.
- *Jacobi is nonetheless a reasonable surrogate for explicit timesteppers*

Complexity Models for Iterative Solvers

- Point Jacobi iteration (7-point stencil, 3D):

- Work:

$$T_{aJ} \sim 14 n/P t_a$$

- Communication:

$$T_{cJ} \sim (6 + (n/P)^{2/3} (1/m_2)) \alpha t_a$$

- Conjugate gradient iteration (7-point stencil): (alt: *Chebyshev iteration*)

- Work:

$$T_{aCG} \sim 27 n/P t_a$$

- Communication:

$$T_{cCG} \sim T_{cJ} + 4 \log_2 P \alpha t_a$$

- Geometric Multigrid:

- Work:

$$T_{aMG} \sim 50 n/P t_a$$

- Communication:

$$T_{cMG} \sim (8 \log_2 n/P + 30/m_2 (n/P)^{2/3} + 8 \log_2 P) \alpha t_a$$

Scaling Estimates: Jacobi

- Q: How large must n/P be for $T_a \sim T_c$?

$$\frac{T_c}{T_a} = \frac{6 \left(1 + \frac{1}{m_2} (n/P)^{2/3} \right) \alpha}{14 n/P} \leq 1$$

$$\left. \begin{array}{l} \alpha = 2300 \\ \beta = 12.6 \\ m_2 = 185 \end{array} \right\} \text{BG/P parameters (BG/Q is similar)}$$

$$(n/P) \approx 2000$$

- Jacobi scaling is independent of P .
 - Of course, need occasional all_reduce to check convergence...
 - Also, *not* a scalable algorithm (but, similar to explicit timestepper)

Scaling Estimates: Conjugate Gradients

$$\underline{z} = D^{-1} \underline{r}$$

$$\underline{r} = \underline{r}^t \underline{z}$$

$$\underline{p} = \underline{z} + \beta \underline{p}$$

$$\underline{w} = A \underline{p}$$

$$\sigma = \underline{w}^t \underline{p}$$

$$\underline{x} = \underline{x} + \alpha \underline{p}$$

$$\underline{r} = \underline{r} - \alpha \underline{p}$$

- The inner-products in CG, which give it its optimality, drive up the minimal effective granularity because of the log P scaling of all_reduce.

Scaling Estimates: Conjugate Gradients

$$\frac{T_c}{T_a} = \frac{6 \left(1 + \frac{1}{m_2} (n/P)^{2/3} + 4 \log_2 P \right) \alpha}{27 n/P} \leq 1$$

$$P = 10^6, \quad \log_2 P = 20,$$

$$(n/P) \approx 8500$$

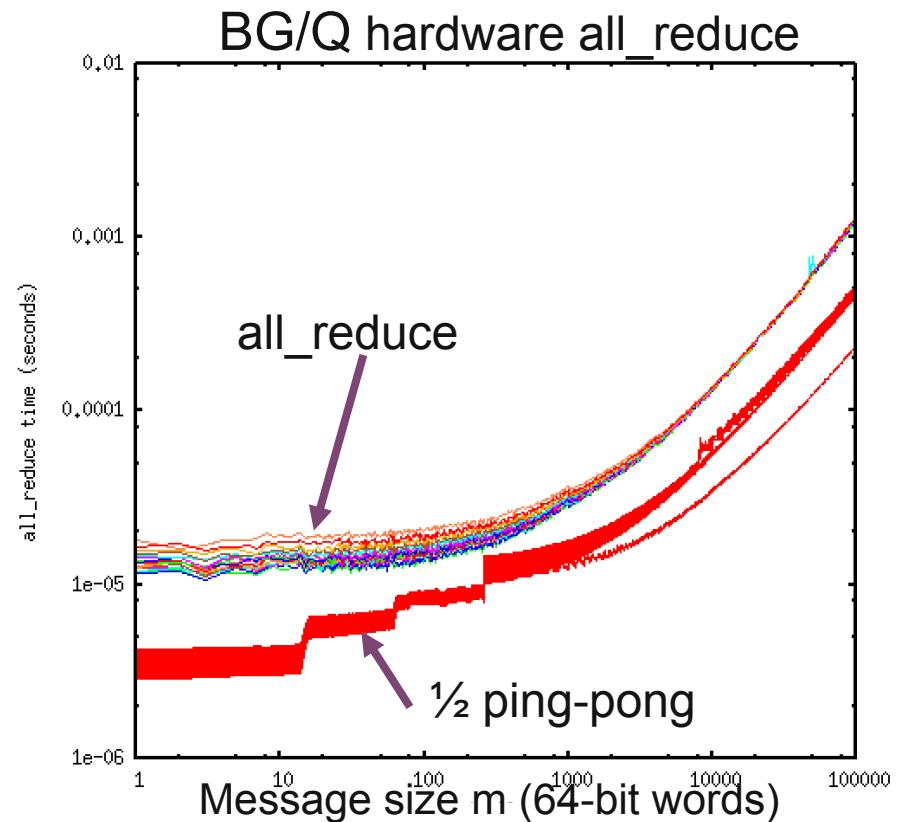
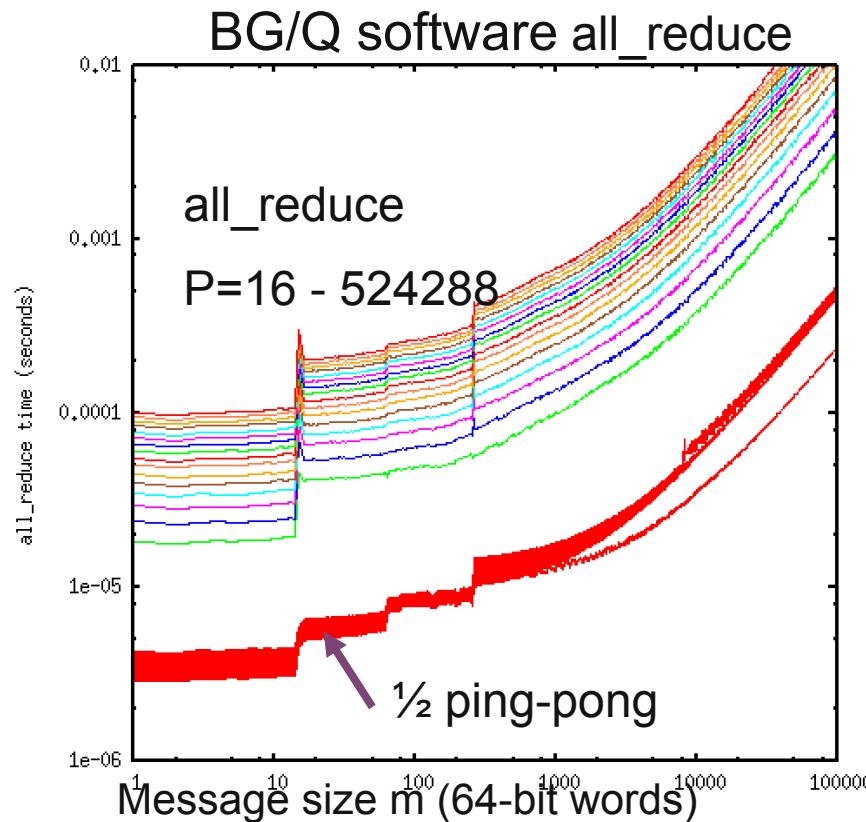
$$P = 10^9, \quad \log_2 P = 30,$$

$$(n/P) \approx 12000$$

- ❑ The inner-products in CG, which give it its optimality, drive up the minimal effective granularity because of the log P scaling of all_reduce.
- ❑ On BG/L, /P, /Q, however, all_reduce is effectively P-independent.

Eliminating log P term in CG

- On BG/L, /P, /Q, all_reduce is nearly ***P-independent***.
- For P=524288, all_reduce(1) is only ***4α*** !



Eliminating log P term in CG

$$\frac{T_c}{T_a} = \frac{6 \left(1 + \frac{1}{m_2} (n/P)^{2/3} + 4 \log_2 P \right) \alpha}{27 n/P} \leq 1$$

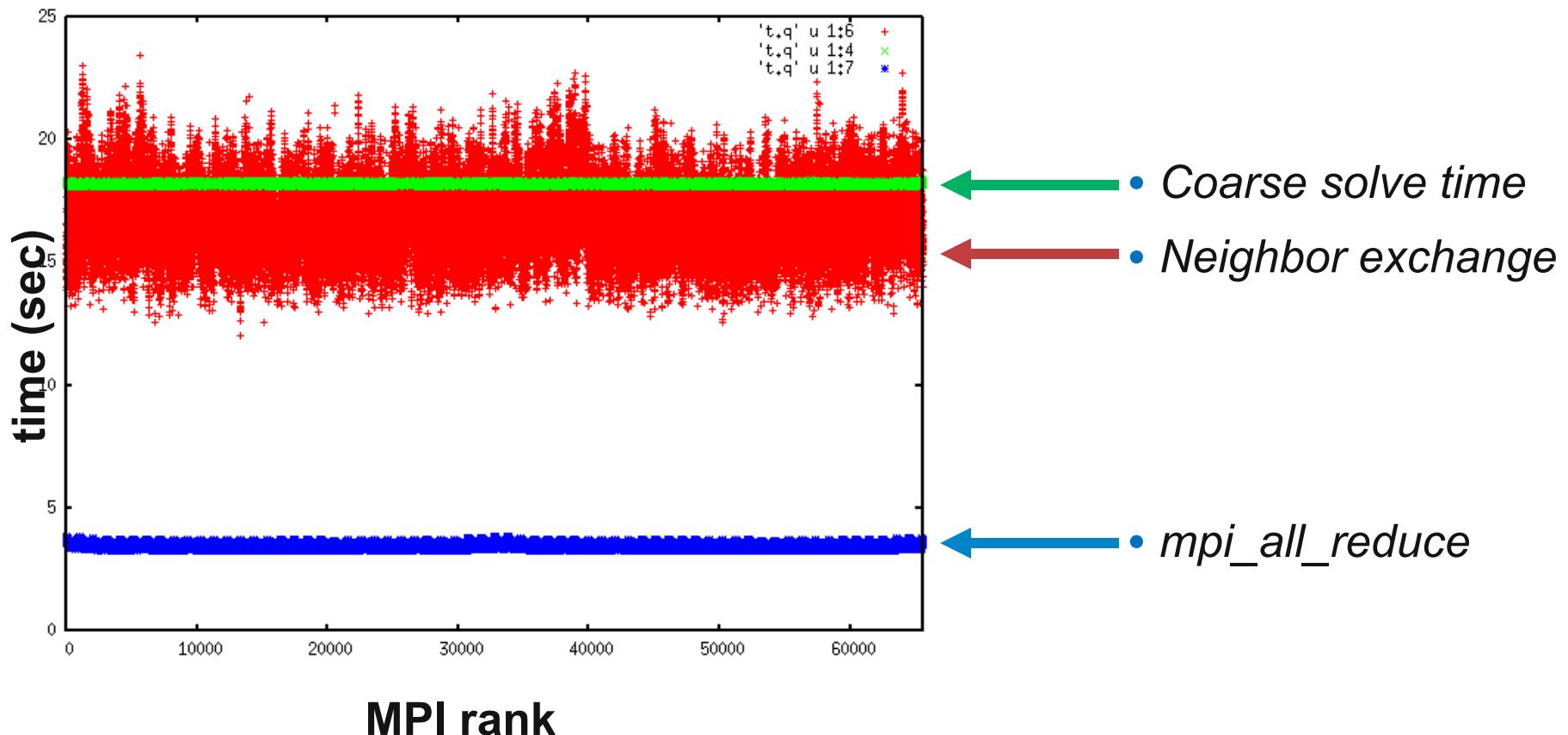
2 x 4 

$$n/P \approx 1200$$

- ❑ On BG/L, /P, /Q, CG is effectively P-independent because of *hardware supported all_reduce*.
- ❑ In this (admittedly simple) exascale model, net result is a 10x improvement in granularity (**n/P=1200 vs. 12,000**).
→ 10x faster run, but no reduction in power consumption.

Nek/BGP Communication Cost Distribution vs Rank

- Billion-point 217-pin bundle simulation on P=65536



- Neighbor vs. all_reduce: 50α vs 4α (4α , not $16 \times 4\alpha$)

Scaling Estimates: Multigrid

$$\frac{T_c}{T_a} = \frac{\left(8 \log_2 n/P + \frac{30}{m_2} (n/P)^{2/3} + 8 \log_2 P\right) \alpha}{50 n/P} \leq 1$$

$$n/P (P = 10^3) \approx 13,000$$

$$n/P (P = 10^6) \approx 17,000$$

$$n/P (P = 10^9) \approx 22,000$$

- Replacing $8 \alpha \log_2 P$ with 16α yields $n / P \sim 9000$, which is $> 2x$ gain in scalability.

Such gains could be realized through hardware support in the network interface card (NIC) for scan / reduce operation

- Some vendors have indicated a move in this direction. (yay!)
- Further savings might be possible by reducing the first term.
(Algorithmic issues addressed by Bell, Dalton, Olson, 2013.)
This is an excellent co-design opportunity.

Measured and Modeled Multigrid Performance

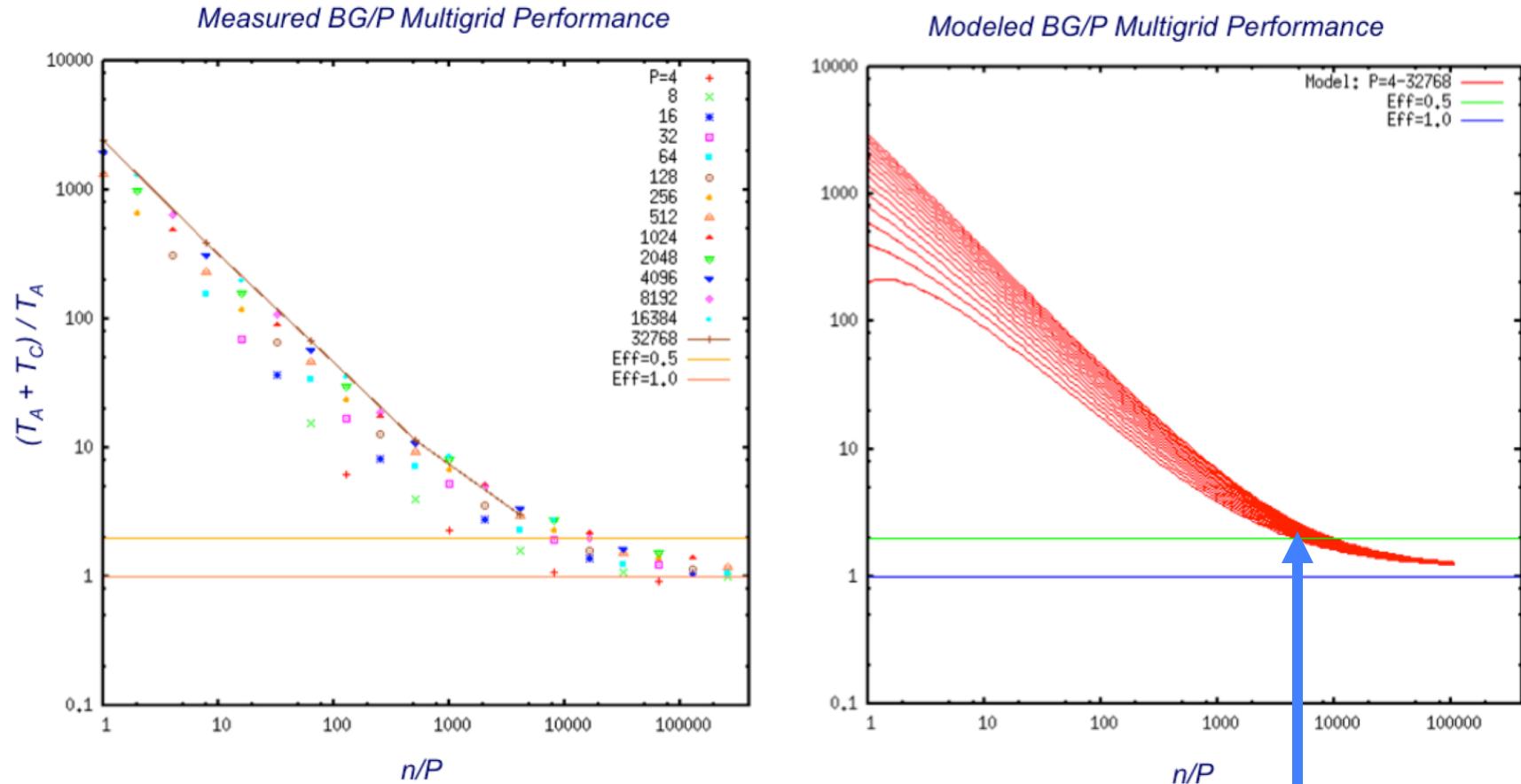


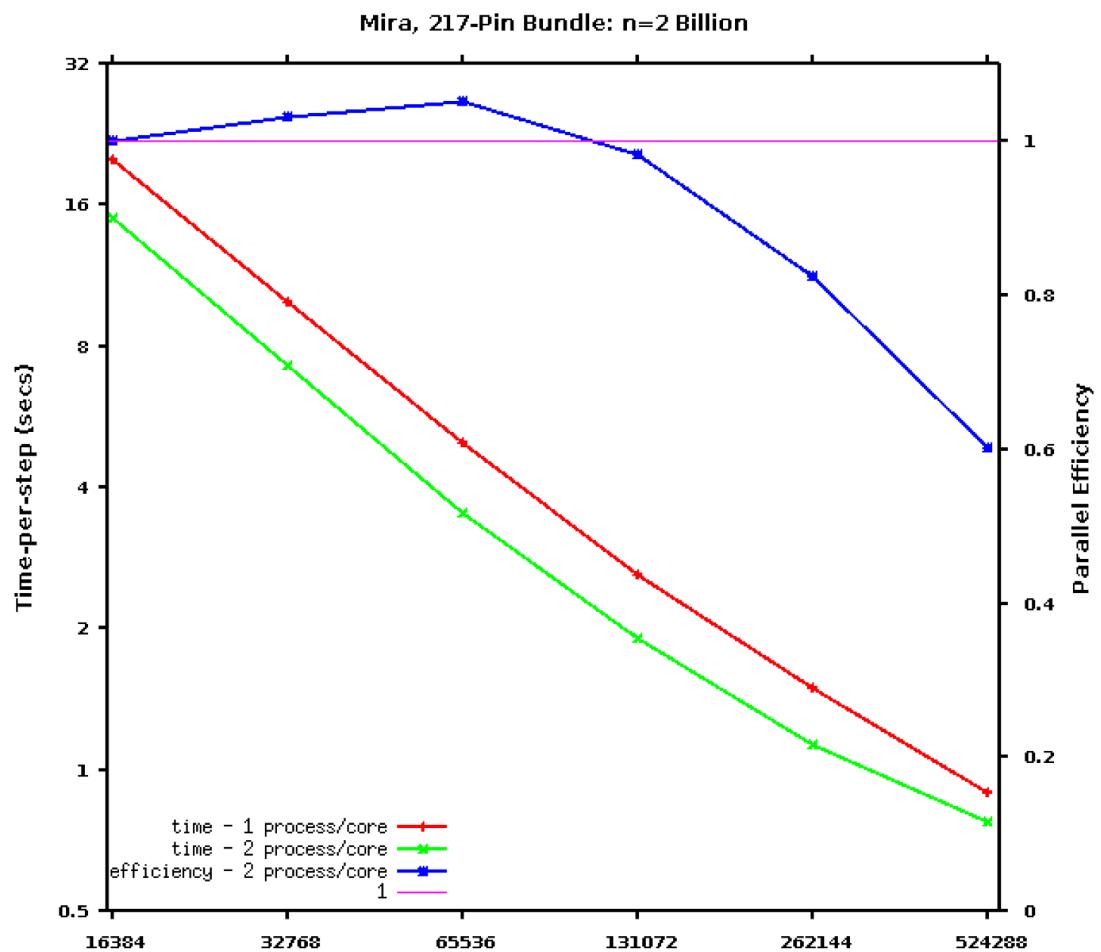
Figure 1.1: Left: Measured scalability for 3D geometric multigrid, $(T_A + T_C)/T_A$ as a function of (number of processor counts, P). Right: Modeled scalability for 3D geometric multigrid using 1.1.

$$T_A = T_C$$

Returning to Original Scaling Question

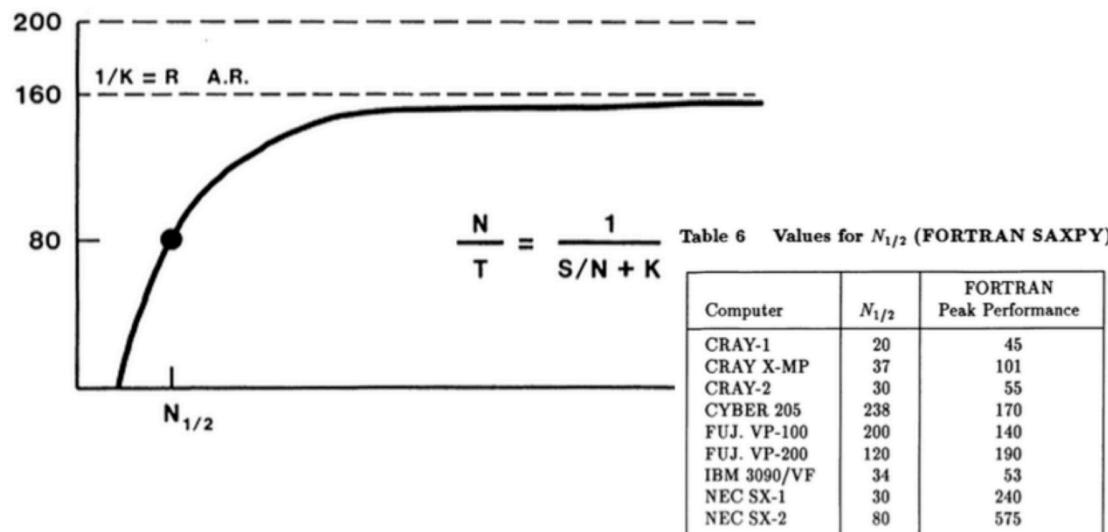
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- BGQ – 524288 cores
 - 1 or 2 ranks per core
- A mixture of CG / multigrid
- 60% parallel efficiency at 1 million processes
- *2000 points/process*



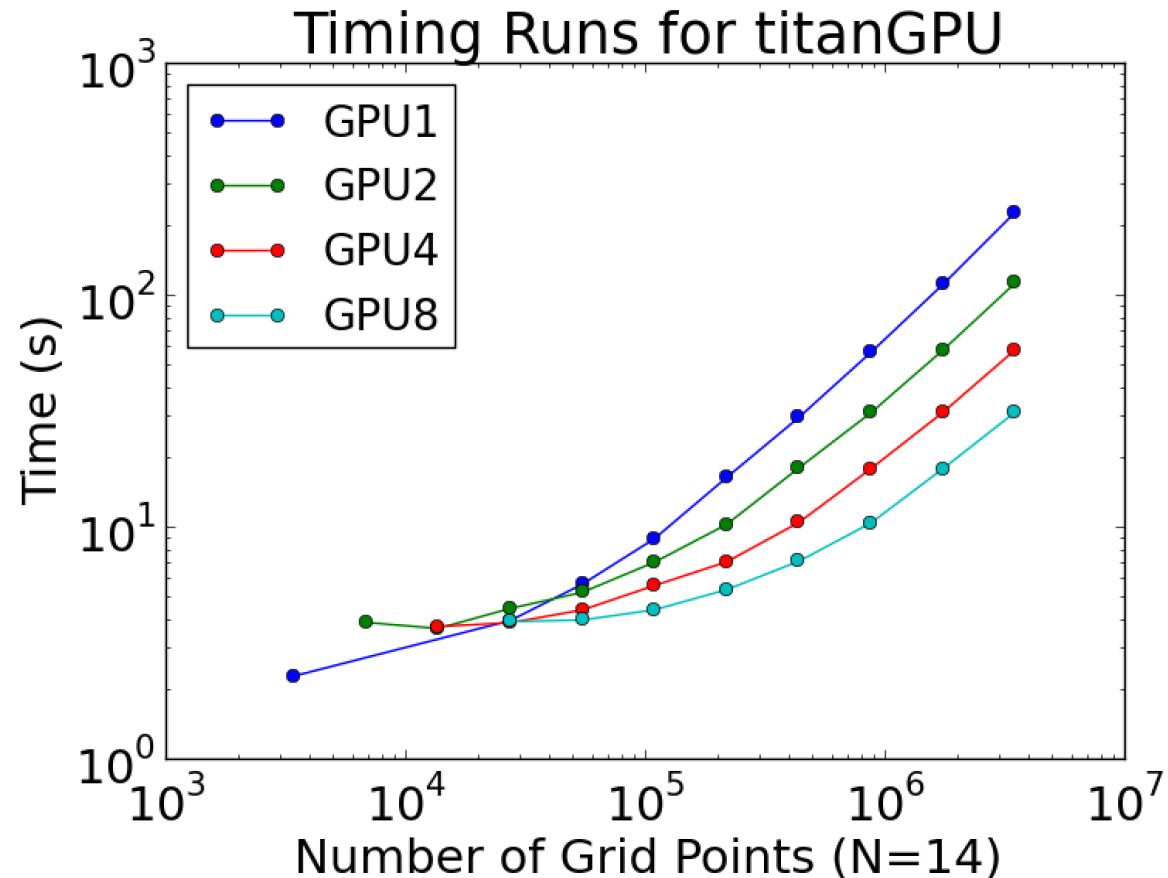
What about GPUs or more Complex Nodes?

- A major concern here is the “ $n_{1/2}$ ”
 - $n_{1/2} :=$ the value of n (or, n/P) where the node performance reaches $\frac{1}{2}$ its peak *for your application*.
- In addition to communication overhead, $n_{1/2}$ sets the strong scale limit on complex nodes.
- This is an old vector-architecture concern that is of critical importance for strong scaling on today and tomorrow’s architectures.



Example of a High $n_{1/2}$

- Electromagnetics code on GPUs of OLCF's Titan.
- Even with P=1, n/P is limited to be > 125,000 to get saturated performance per node (for CFD, this number is higher).



$n_{1/2}$ Requirements for a Candidate Node to Yield Speedup

$$S_P = \eta \cdot S_1 \cdot P \quad (\text{speed, in mflops})$$

S_1 = observed saturated speed, in flops, $n \gg 1$

- Let n be total problem size (gridpoints, say), and $n_{\frac{1}{2}}$ be the local problem size such that

$$S_1(n_{\frac{1}{2}}) = \frac{1}{2}S_1(n_{\text{sat}})$$

- Let $W := w \cdot n$ be the total number of flops and w be the number of flops per gridpoint.
- Choose $P = n/n_{\frac{1}{2}}$ (50% efficiency)

- Time to solution:
$$\begin{aligned} T_P &= \frac{w \cdot n}{S_P} = \frac{w \cdot n}{\eta S_1 P} \\ &= \frac{w \cdot n}{\eta S_1(n/n_{\frac{1}{2}})} = \frac{w \cdot n_{\frac{1}{2}}}{\frac{1}{2}S_1} \\ &= 2w \left(\frac{n_{\frac{1}{2}}}{S_1} \right) \end{aligned}$$

Summary: Getting Good Performance for CFD, PDEs, HPC

- Know your model & physics (if possible):
 - RANS vs LES – 10^4 – 10^5 savings
- PDEs:
 - Discretizations can yield 10x savings
 - Fast solvers 10-100x
- HPC:
 - Understand your single-node performance, over a range of n!
 - Examine your communication costs.
 - All of this involves modeling and measuring.
- The HPC part can be almost (!) as much fun as the fluids part!

Thank You!

