

Efficient Numerical Simulation of Advection Diffusion Systems

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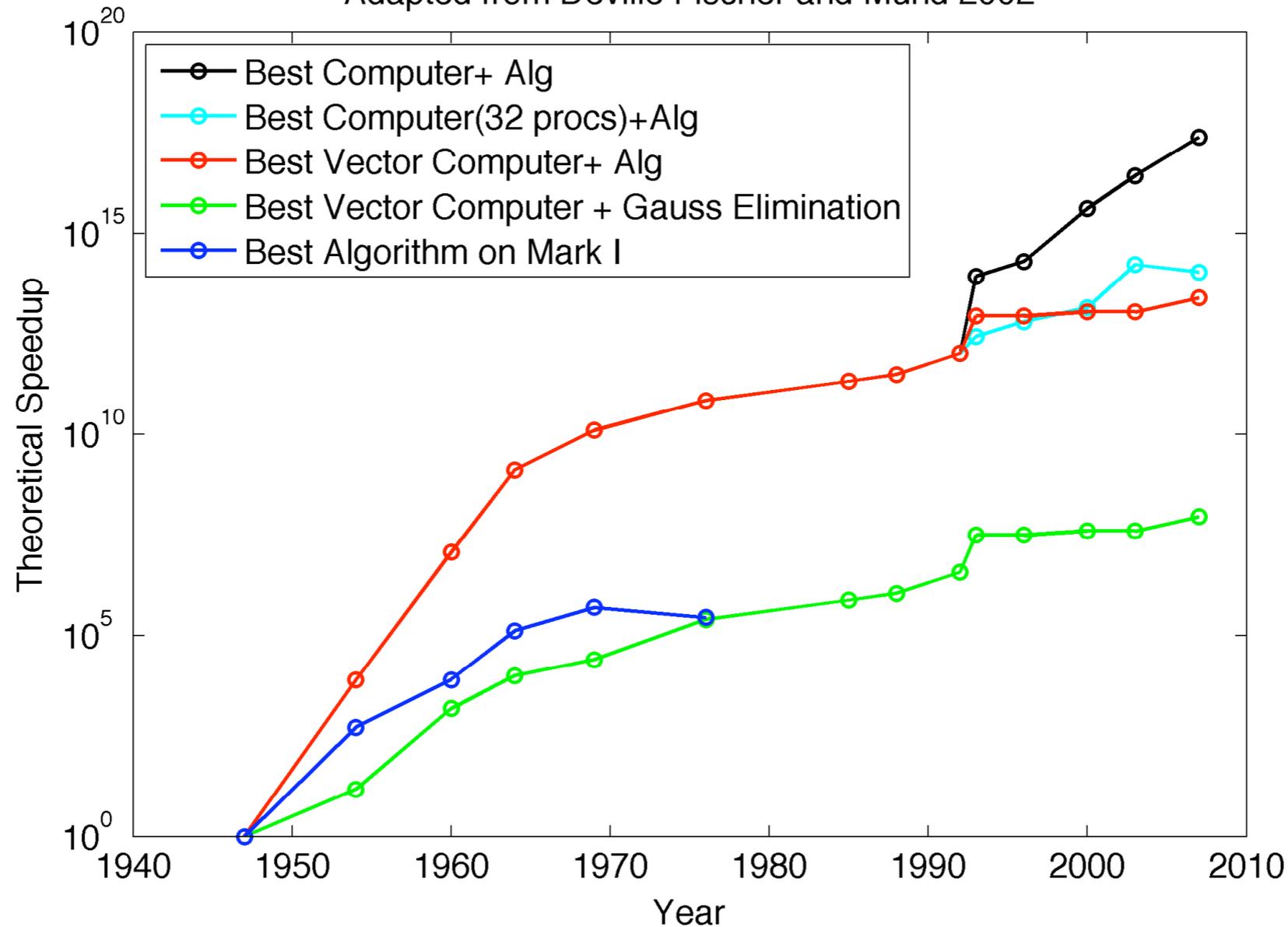
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OUTLINE

- **History of machine and algorithmic speedup**
- **Introduction to Advection-Diffusion Systems**
- **Choice of Numerical Discretization**
- **Development of Numerical Solvers**
- **Results**
- **Conclusion/Future Directions**

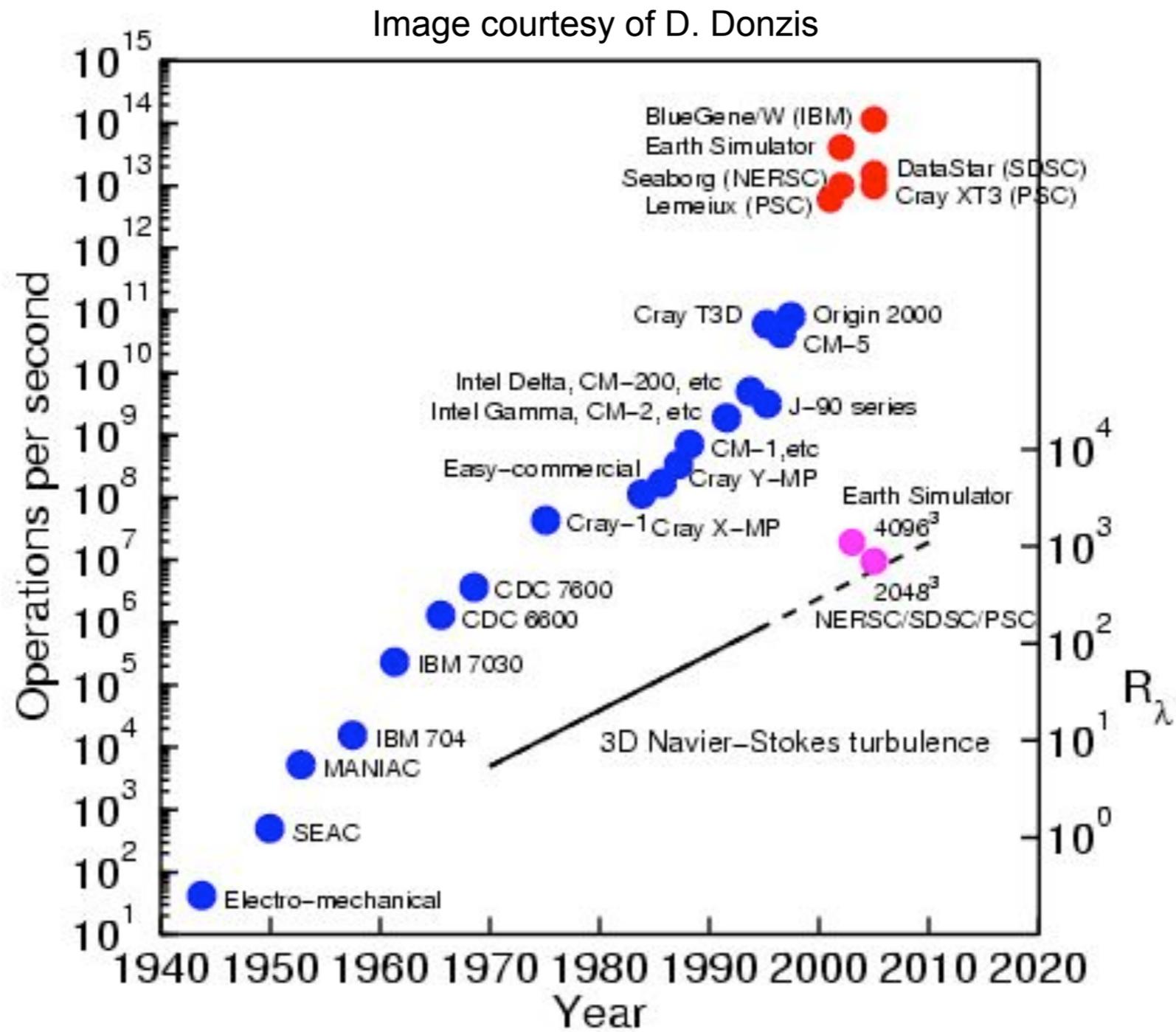
Motivation - Efficient Solvers

Evolution of machines, algorithms and their combination
over the past 60 years for the solution of a 3D Poisson Eqn
Adapted from Deville Fischer and Mund 2002



Faster machines and computational algorithms
can dramatically reduce simulation time.
(Centuries to milliseconds).

Motivation - Efficient Solvers



Simulating complex flows doesn't scale as well.

Motivation - Efficient Solvers

Complexity of Modern Linear Solvers

		Serial	Parallel
FFT	Direct	$n \log n$	$\log n$
Multigrid	Iterative	n	$(\log n)^2$
GMRES	Iterative	n	n
Lower Bound		n	$\log n$

Model - Steady Advection Diffusion

$$-\epsilon \nabla^2 u + (\vec{w} \cdot \nabla) u = f$$

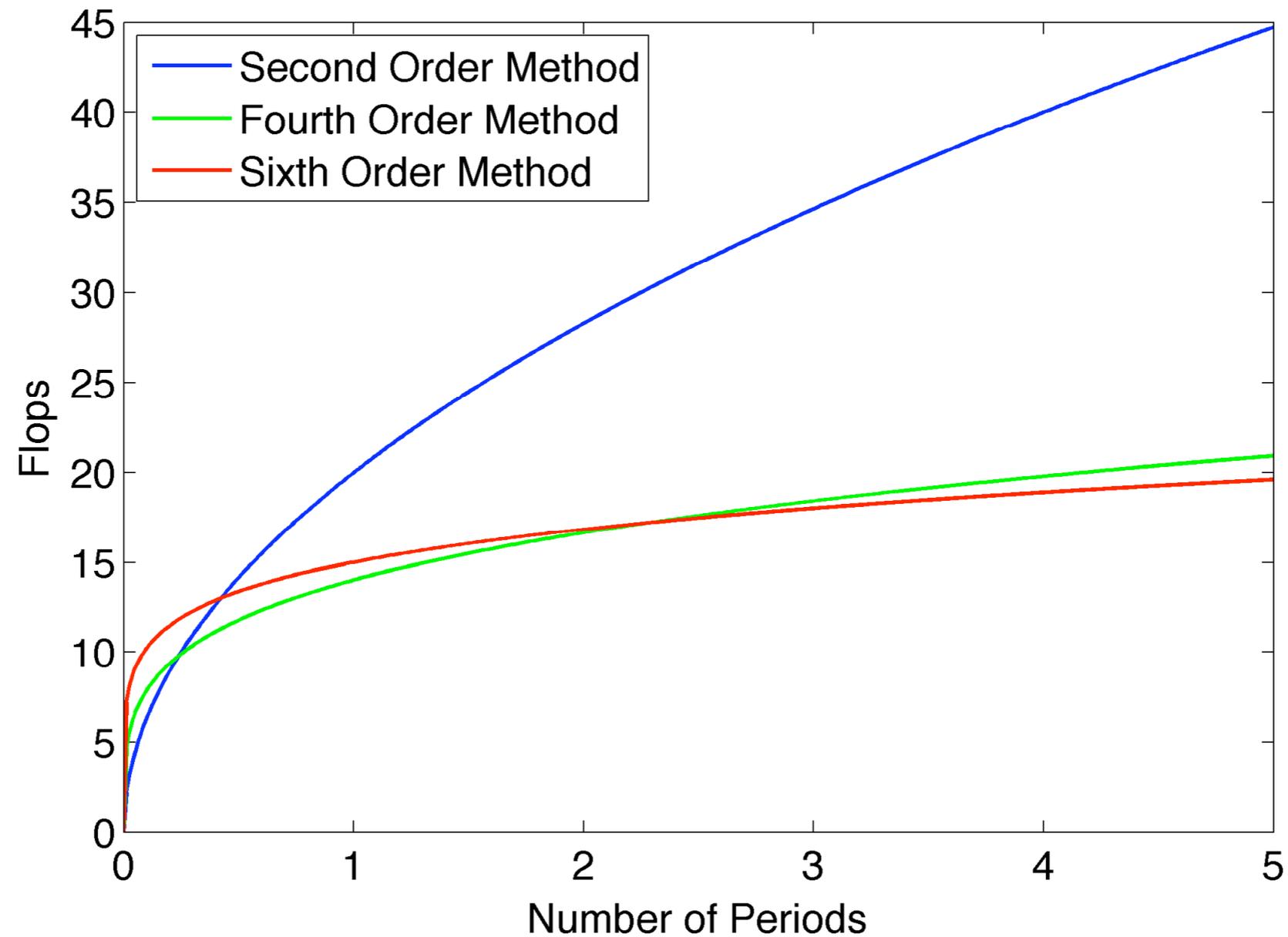
Inertial and viscous forces occur on disparate scales causing **sharp flow features** which:

- require fine numerical grid resolution
- cause poorly conditioned non-symmetric discrete systems.

These properties make solving the discrete systems **computationally expensive**.

Motivation - Efficient Solvers & Discretization

Comparison of computational work needed to maintain
10% phase error in 1D advection equation
Karniadakis & Sherwin 2005

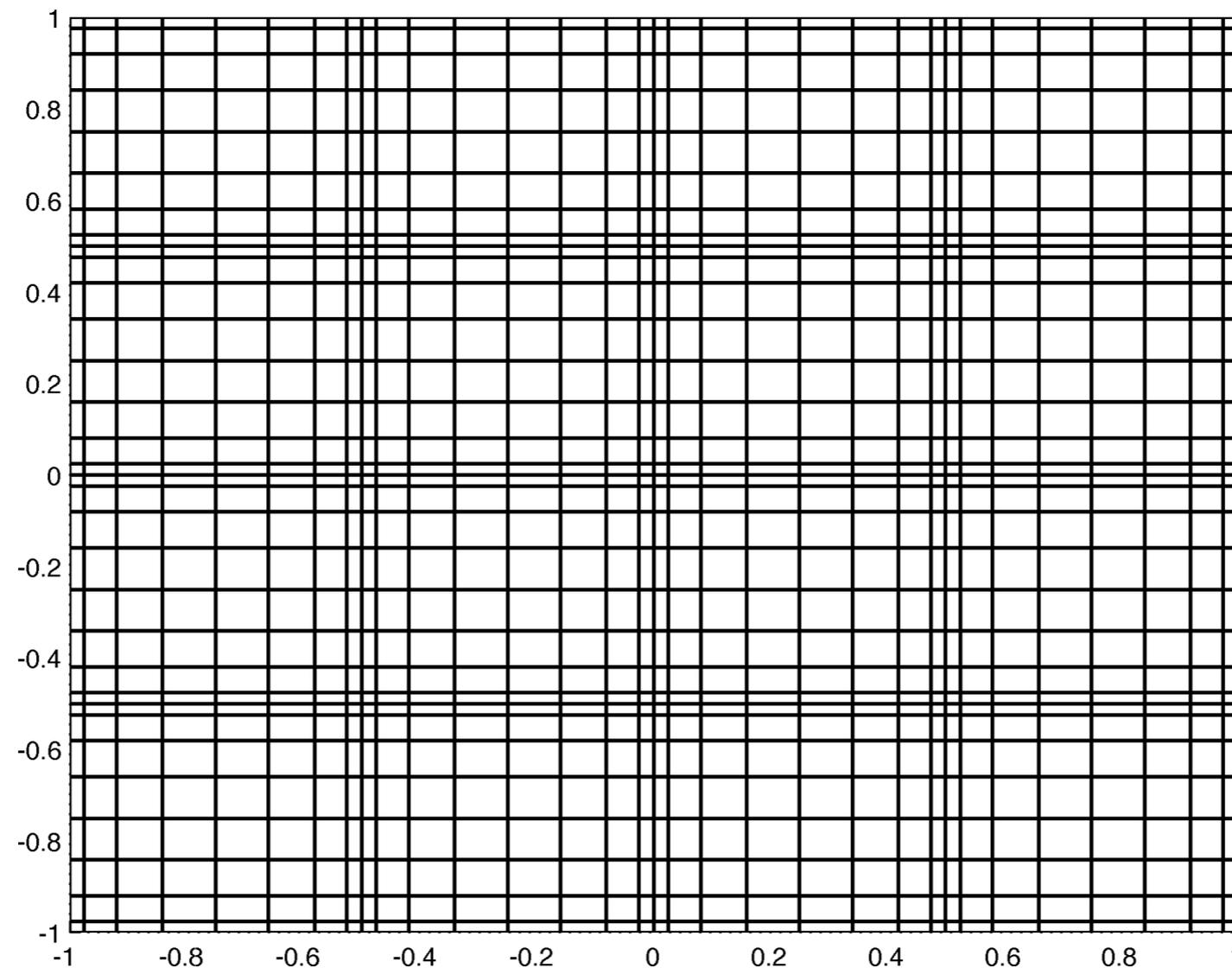


High order methods are accurate & efficient.

Methods - Spectral Element Discretization

Spectral elements provide:

- **flexible geometric boundaries**
- **large volume to surface ratio**
- **low storage requirements**



The discrete system of advection-diffusion equations are of the form:

$$F(\vec{w})u = Mf$$

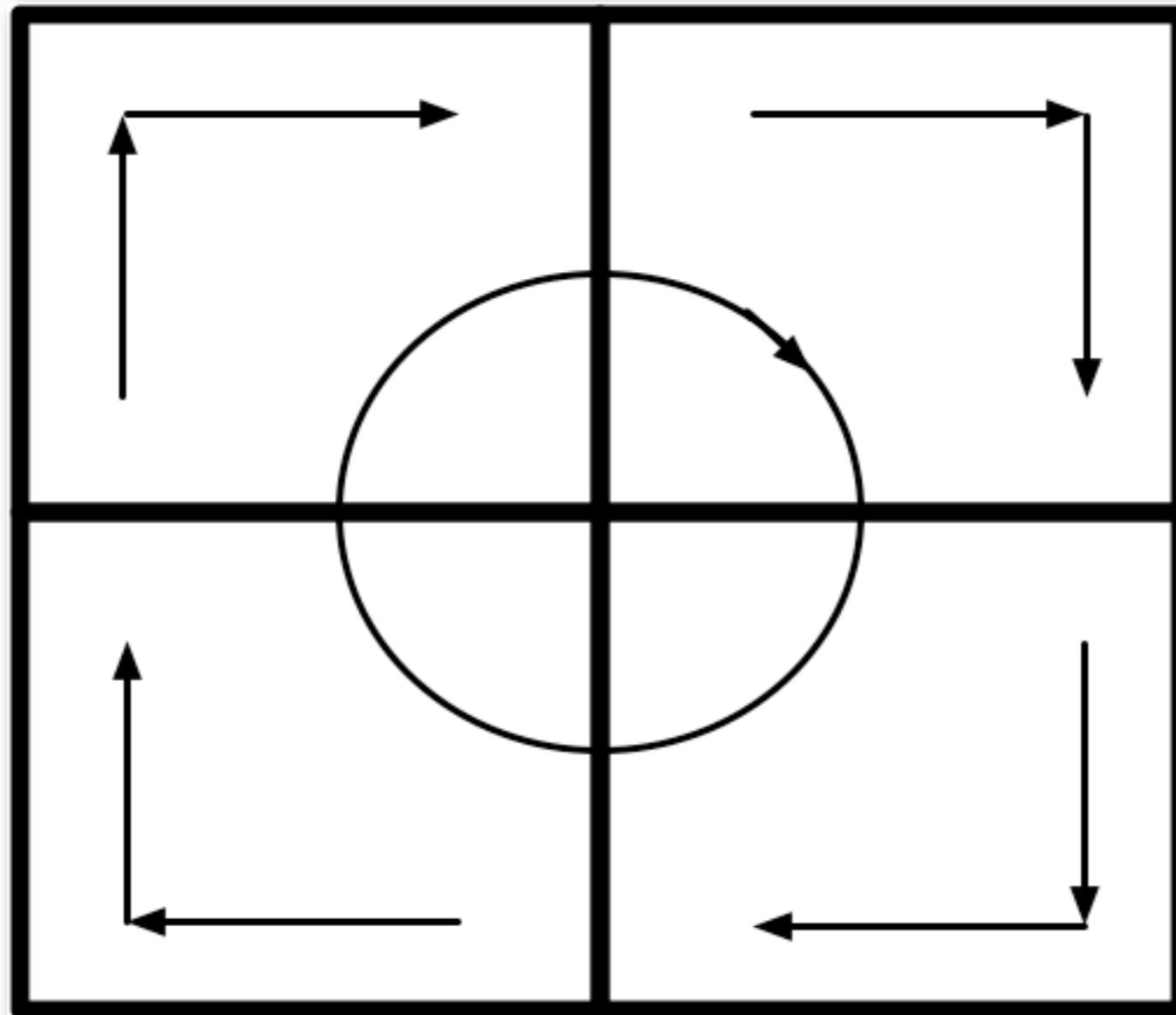
When w is constant in each direction on each element we can use

- **Fast Diagonalization & Domain Decomposition as a solver.**

$$\tilde{F} = \hat{M} \otimes \hat{F}(w_x) + \hat{F}(w_y) \otimes \hat{M}$$

Otherwise, we can use this as a **Preconditioner** for an iterative solver such as GMRES

$$F(\vec{w})P_F^{-1}P_F u = M f$$



What does \otimes mean?

Suppose $A_{k \times l}$ and $B_{m \times n}$

The Kronecker Tensor Product

$$C_{km \times ln} = A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \dots & a_{1l}B \\ a_{21}B & a_{22}B & \dots & a_{2l}B \\ \vdots & \vdots & & \vdots \\ a_{k1}B & a_{k2}B & \dots & a_{kl}B \end{pmatrix}.$$

Matrices of this form have properties that make computations **very efficient** and **save lots of memory!**

Methods - Fast Diagonalization

Matrix-vector multiplies $(A \otimes B)\vec{u} = BU A^T$
done in $O(n^3)$ flops instead of $O(n^4)$

Fast Diagonalization Property

$$C = A \otimes B + B \otimes A$$

$$V^T A V = \Lambda, \quad V^T B V = I$$

$$C = (V \otimes V)(I \otimes \Lambda + \Lambda \otimes I)(V^T \otimes V^T)$$

$$C^{-1} = (V \otimes V)(I \otimes \Lambda + \Lambda \otimes I)^{-1}(V^T \otimes V^T)$$

Only need an inverse of a **diagonal matrix!**

We use Flexible GMRES with a **preconditioner** based on:

- **Local constant wind approximations**
- **Fast Diagonalization**
- **Domain Decomposition**

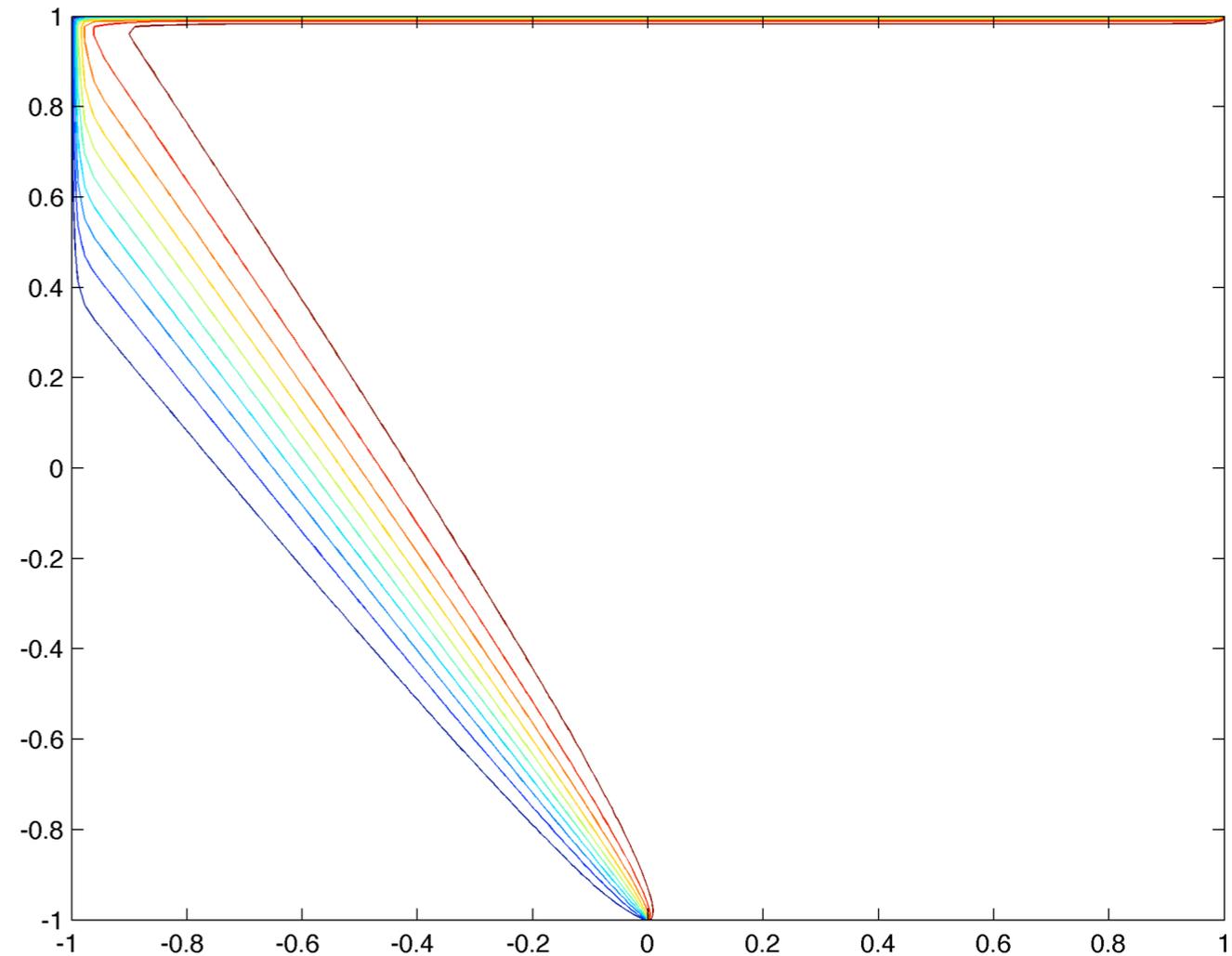
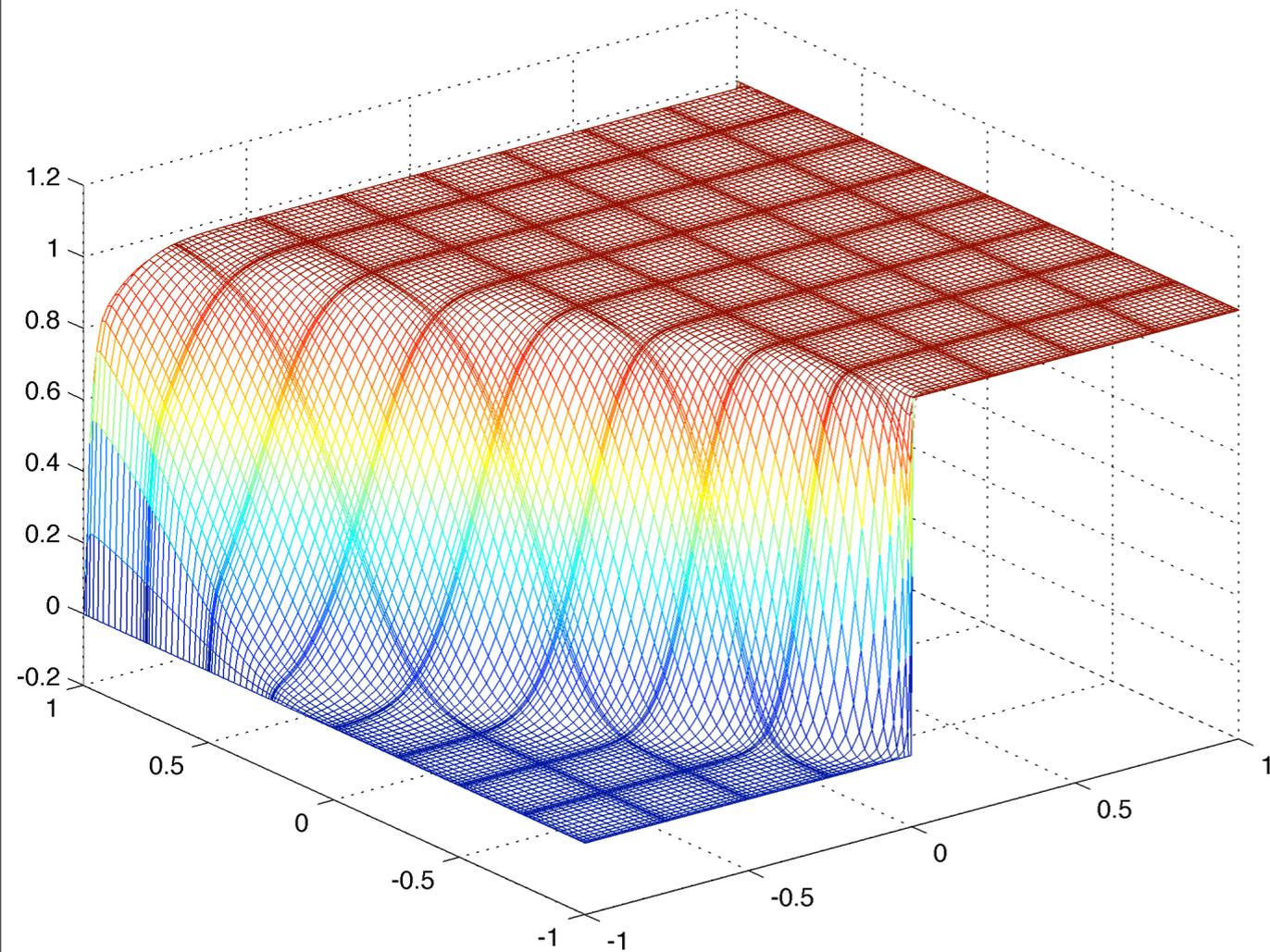
$$F(\vec{w}) P_F^{-1} P_F u = M f$$

$$P_F^{-1} = R_0^T \tilde{F}_0^{-1}(\bar{w}_0) R_0 + \sum_{e=1}^N R_e^T \tilde{F}_e^{-1}(\bar{w}^e) R_e$$

$$\tilde{F}_e^{-1} = (\hat{M}^{-1/2} \otimes \hat{M}^{-1/2})(S \otimes T)(\Lambda \otimes I + I \otimes V)^{-1}(S^{-1} \otimes T^{-1})(\hat{M}^{-1/2} \otimes \hat{M}^{-1/2})$$

Solver Results - Constant Wind

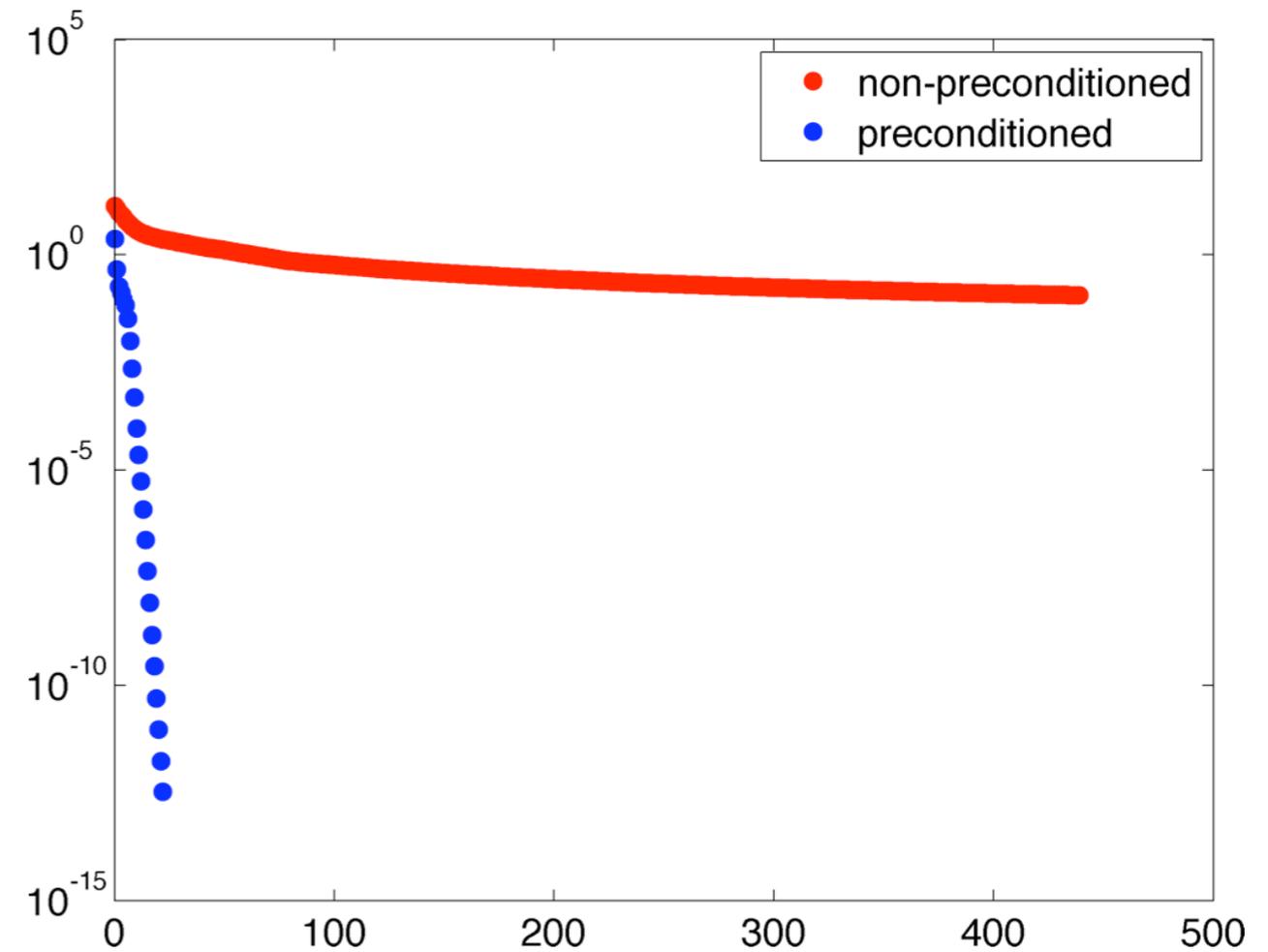
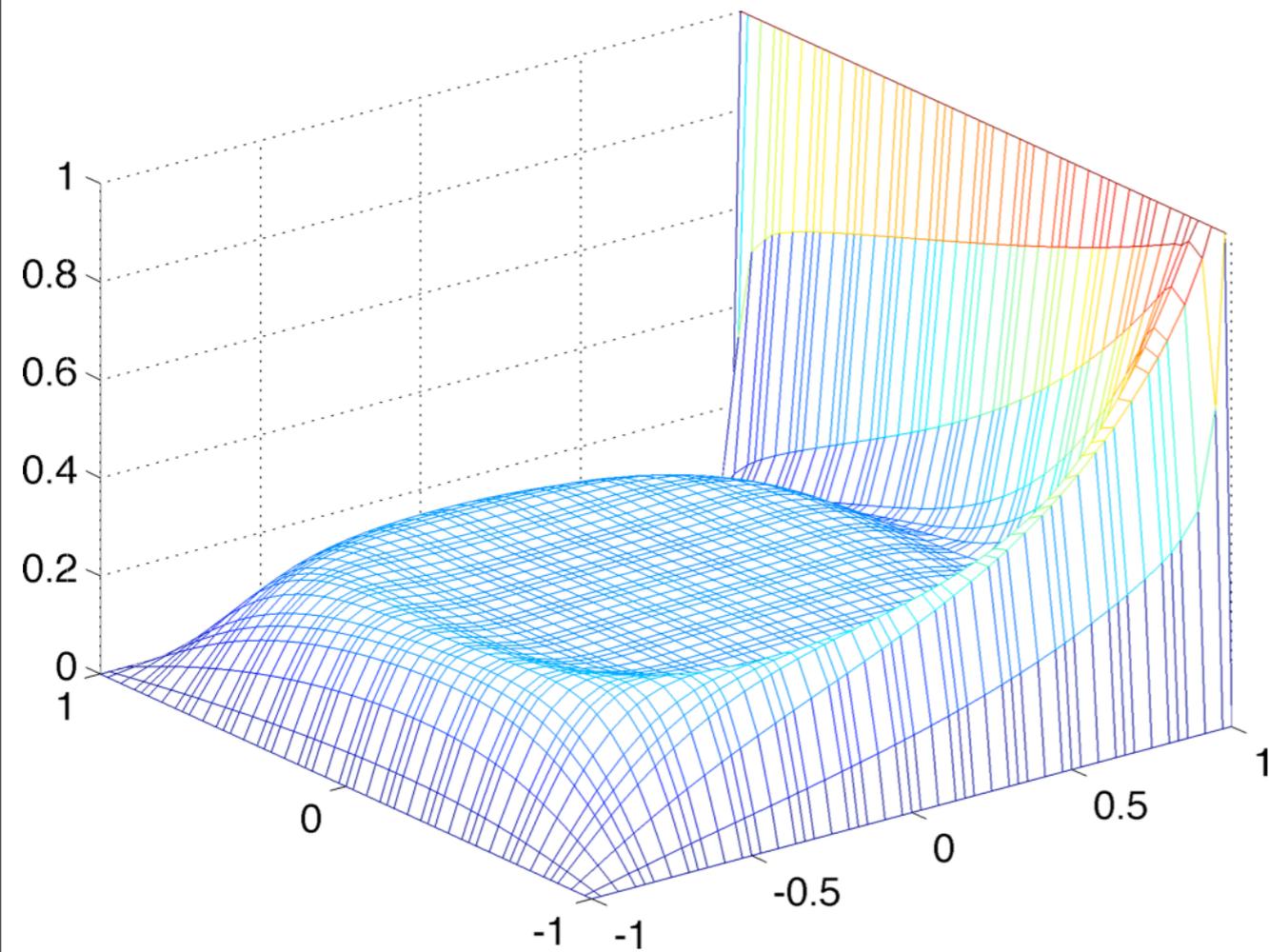
$$\vec{w} = 200\left(-\sin\left(\frac{\pi}{6}\right), \cos\left(\frac{\pi}{6}\right)\right)$$



Solution and contour plots of a steady advection-diffusion flow. Via Domain Decomposition & Fast Diagonalization. Interface solve takes 150 steps to obtain 10^{-5} accuracy.

Preconditioner Results - Recirculating Wind

$$\vec{w} = 200(y(1 - x^2), -x(1 - y^2))$$



Hot plate at wall forms internal boundary layers.

Residual Plot above.

• $(P + 1) [120N + (P + 1)]$
additional flops per step

Coupling Fast Diagonalization & Domain Decomposition provides an efficient solver for the advection-diffusion equation.

- Precondition Interface Solve
- Coarse Grid Solve (multilevel DD)
- Multiple wind sweeps
- Time dependent flows
- 2D & 3D Navier-Stokes
- Apply to study of complex flows

References

M. Deville, P. Fischer, E. Mund, High-Order Methods for Incompressible Fluid Flow, Cambridge Monographs on Applied and Computational Mathematics, 2002.

H. Elman, D. Silvester, & A. Wathen, Finite Elements and Fast Iterative Solvers with applications in incompressible fluid dynamics, Numerical Mathematics and Scientific Computation, Oxford University Press, New York, 2005.

H. Elman, P.A. Lott Matrix-free preconditioner for the steady advection-diffusion equation with spectral element discretization. In preparation. 2008.