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An Overview of Automatic Differentiation and Introduction to the OpenAD/F Tool

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Funding

- Current:
  - DOE: Applied Mathematics Base Program
  - DOE: Computer Science Base Program
  - DOE: CSCAPES SciDAC Institute
  - NASA: ECCO-II Consortium
  - NSF: Collaborations in Math & Geoscience
- Past:
  - DOE: Applied Math
  - NASA Langley
  - NSF: ITR

Outline

- Introduction to automatic differentiation (AD)
- AD in nuclear systems modeling
- Computing derivatives efficiently under various scenarios
- Ideas for computing very large, very dense Jacobians efficiently
- Survey of available tools
- Application examples
- Handoff to Utke for discussion of OpenAD/F and its application to SCALE

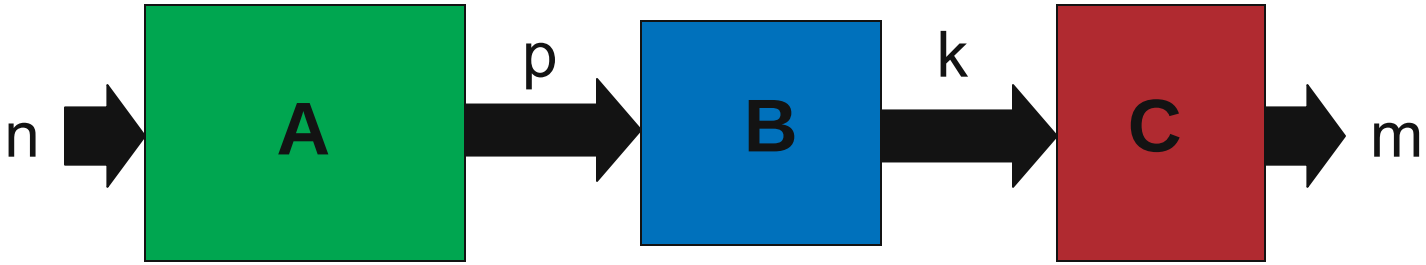
Automatic Differentiation in a Nutshell

- Technique for computing analytic derivatives of programs (millions of loc)
- Derivatives used in optimization, sensitivity analysis, inverse problems, …
- AD = analytic differentiation of elementary functions + propagation by chain rule
  - Every programming language provides a limited number of elementary mathematical functions
  - Thus, every function computed by a program may be viewed as the composition of these so-called intrinsic functions
  - Derivatives for the intrinsic functions are known and can be combined using the chain rule of differential calculus
- Associativity of the chain rule leads to two main modes: forward and reverse (adjoint)
- Can be implemented using source transformation or operator overloading

Automatic Differentiation in Nuclear System Modeling

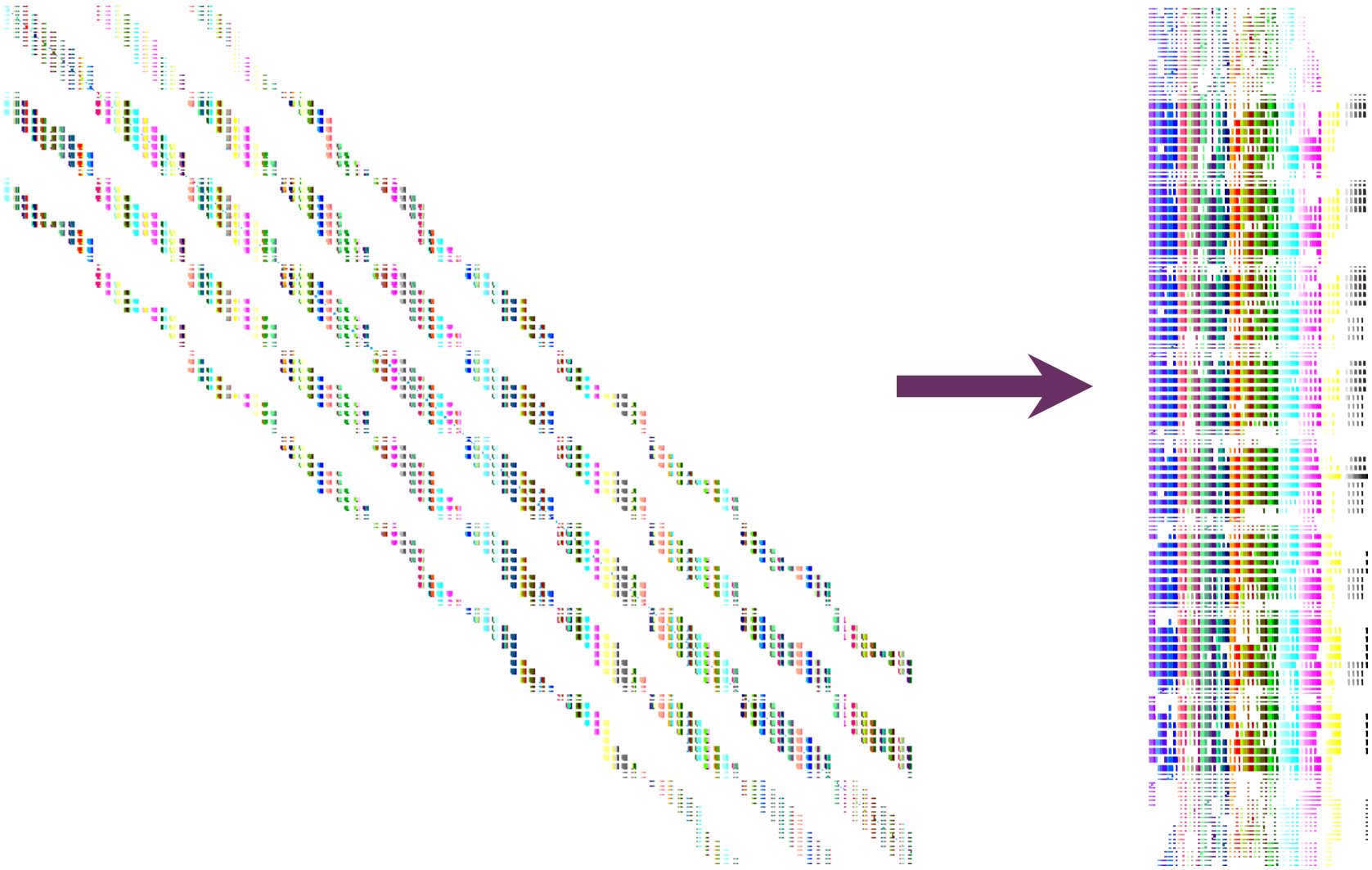
- Derivatives used for:
  - Local sensitivity analysis
  - Construction of first- and second-order Taylor models
  - Providing weights for adaptive sampling
  - Other applications??
- What is feasible & practical
  - Jacobians of functions with small number (1—1000) of independent variables (forward mode)
  - Jacobians of functions with small number (1—100) of dependent variables (adjoint mode)
  - Very (extremely) large, but (very) sparse Jacobians and Hessians (forward mode plus coloring)
  - Jacobian-vector products (forward mode)
  - Transposed-Jacobian-vector products (adjoint mode)
  - Hessian-vector products (forward + adjoint modes)

Scenarios



- N small: use forward mode on full computation
- M small: use reverse mode on full computation
- M & N large, P small: use reverse mode on A, forward mode on B&C
- M & N large, K small: use reverse mode on A&B, forward mode on C
- N, P, K, M large, Jacobians of A, B, C sparse: compressed forward mode
- N, P, K, M large, Jacobians of A, B, C low rank: scarce forward mode

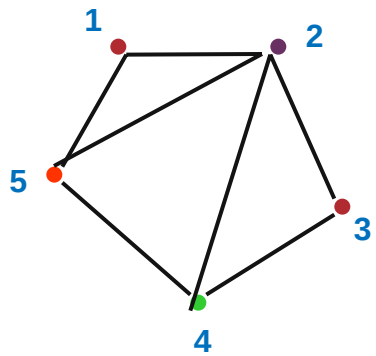
Compressed Jacobian: choose S and compute JS

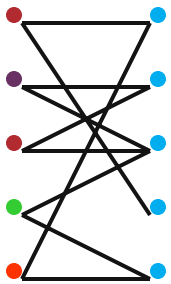


Matrix Coloring (used to determine S)

$$\begin{matrix} 1 & 2 & 0 & 0 & 5 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 2 & 3 & 4 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 5 \end{matrix}$$

$$\begin{matrix} 1 & 2 & 0 & 0 & 5 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 2 & 3 & 4 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 5 \end{matrix} \longrightarrow \begin{matrix} 1 & 2 & 0 & 5 \\ 3 & 0 & 0 & 0 \\ 3 & 2 & 4 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 4 & 5 \end{matrix}$$





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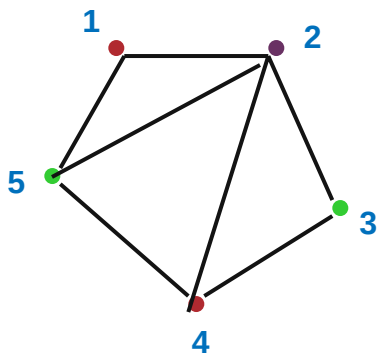

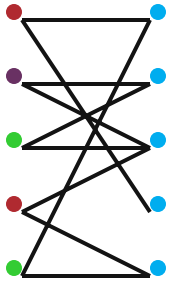

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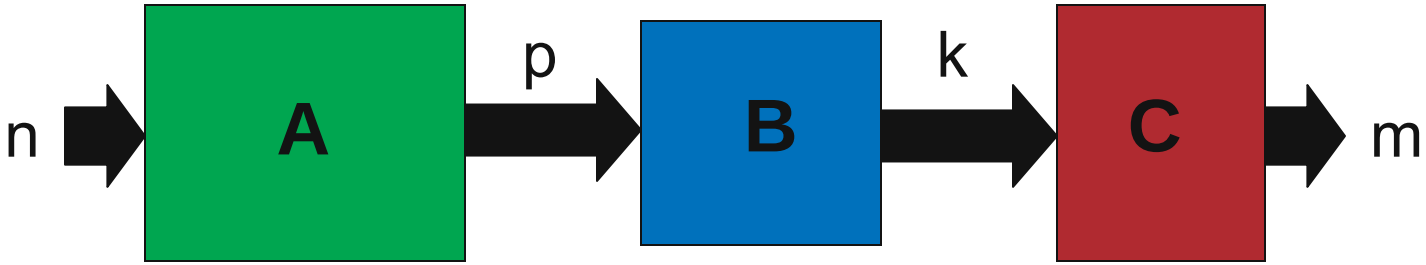

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- **N, P, K, M large: Jacobians of A, B, C dense: what to do?**

What to do for very large, dense Jacobian matrices?

- Jacobian matrix might be large and dense, but "effectively sparse"
  - Many entries below some threshold ε ("almost zero")
  - Can tolerate errors up to δ in entries greater than ε
  - Example: advection-diffusion for finite time step: nonlocal terms fall off exponentially
  - Solution: do a partial coloring to compress this dense Jacobian: requires solving a modified graph coloring problem
- Jacobian might be large and dense, but "effectively low rank"
  - Can be well approximated by a low rank matrix
  - Jacobian-vector products (and $J^T v$) are cheap
  - Adapt techniques based on sampling of F or finite difference approximations to Jv, $[F(x+hv) - F(x)]/h$
  - One candidate: SVD of random Jacobian-vector products (adaptation of efficient subspace method--joint work with Abdel-Khalik)

Tools

- Fortran 95
- C/C++
- Fortran 77
- MATLAB

Tools: Fortran 95

- TAF (FastOpt)
  - Commercial tool
  - Support for (almost) all of Fortran 95
  - Used extensively in geophysical sciences applications
- Tapenade (INRIA)
  - Support for many Fortran 95 features
  - Developed by a team with extensive compiler experience
- **OpenAD/F (Argonne/UChicago/Rice) – more later**
  - Support for many Fortran 95 features
  - Developed by a team with expertise in combinatorial algorithms, compilers, software engineering, and numerical analysis
  - Development driven by climate model & astrophysics code
- All three: forward and reverse; source transformation

Tools: C/C++

- ADOL-C (Dresden/Humboldt)
  - Mature tool
  - Support for all of C++
  - Operator overloading; forward and reverse modes
- ADIC (Argonne/UChicago)
  - Support for all of C, some C++
  - Source transformation; forward mode (reverse under development)
  - New version (2.0) based on industrial strength compiler infrastructure
  - Shares some infrastructure with OpenAD/F
- TAC++ (FastOpt)
  - Commercial tool (under development)
  - Support for much of C/C++
  - Source transformation; forward and reverse modes
  - Shares some infrastructure with TAF

Tools: Fortran 77

- ADIFOR (Rice/Argonne)
  - Mature and very robust tool
  - Support for all of Fortran 77
  - Forward and (adequate) reverse modes
  - Hundreds of users; ~150 citations

Tools: MATLAB

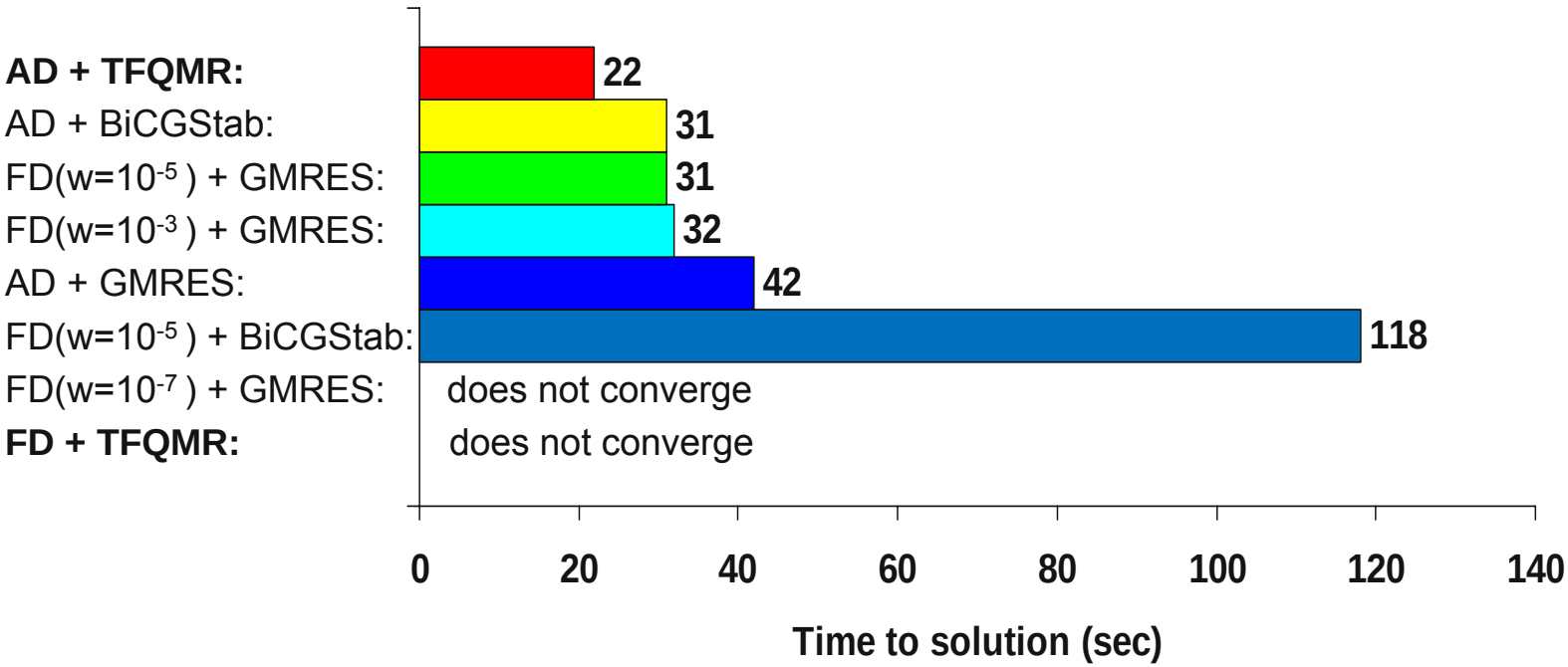
- AdiMat (Aachen): source transformation
- MAD (Cranfield/TOMLAB): operator overloading
- Various research prototypes

Applications

- Nonlinear solver (importance of analytic derivatives)
- Mesh smoothing (potential for automatic code to outperform hand coding)
- Simplified climate model (importance of reverse mode and compiler analysis)

Application: solution of nonlinear PDEs

- Jacobian-free Newton-Krylov solution of model problem (driven cavity)



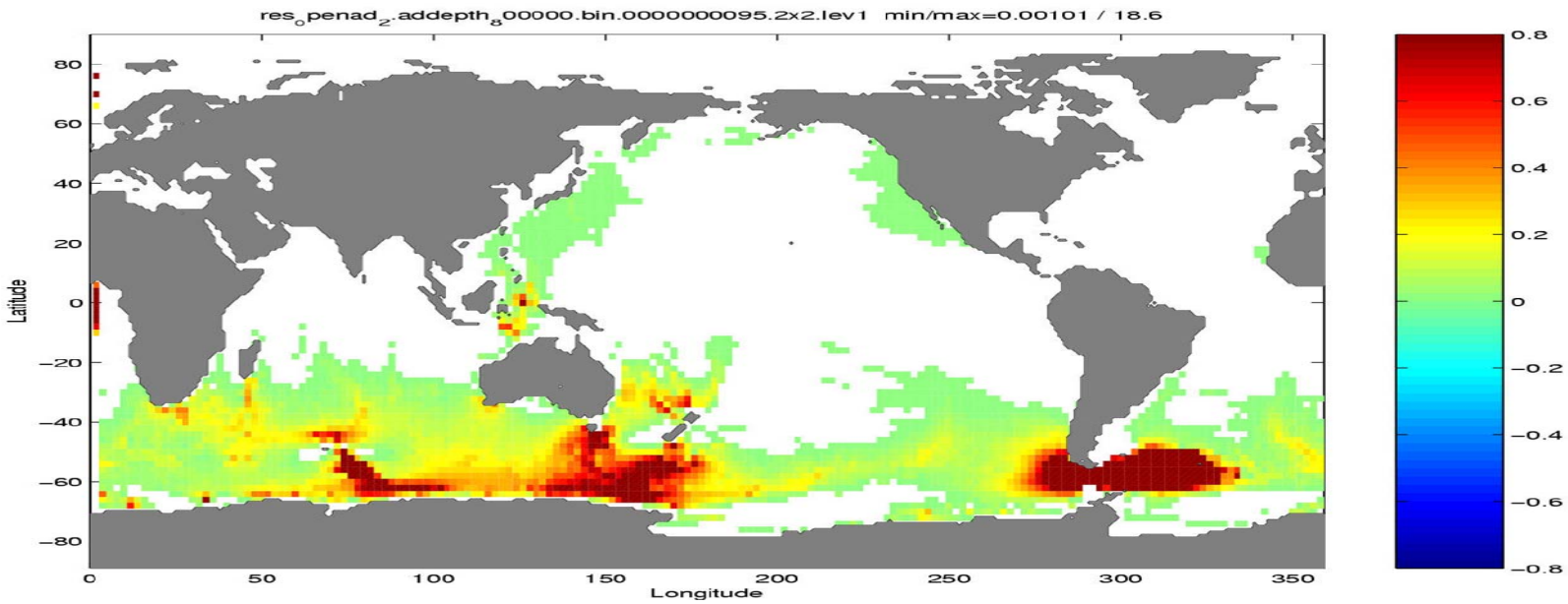
AD = automatic differentiation

FD = finite differences

W = noise estimate for Brown-Saad

Application: Sensitivity analysis in simplified climate model

- Sensitivity of flow through Drake Passage to ocean bottom topography
  - Finite difference approximations: 23 days
  - Naïve automatic differentiation: 2 hours 23 minutes
  - Smart automatic differentiation: 22 minutes



For More Information

- Andreas Griewank, *Evaluating Derivatives*, SIAM, 2000.
- Griewank, “On Automatic Differentiation”; this and other technical reports available online at: http://www.mcs.anl.gov/autodiff/tech_reports.html
- AD in general: http://www.mcs.anl.gov/autodiff/, http://www.autodiff.org/
- ADIFOR: http://www.mcs.anl.gov/adifor/
- ADIC: http://www.mcs.anl.gov/adic/
- OpenAD: http://www.mcs.anl.gov/openad/
- Other tools: http://www.autodiff.org/
- E-mail: hovland@mcs.anl.gov