Finite Difference Approximation

- Solving the problem numerically → transform the continuous problem into a discrete one by:
  - Looking at finite time/space steps
- Assuming all functions are sufficiently smooth, a straightforward Taylor expansion gives:

$$u(t+\Delta t) = u(t) + u'(t)\Delta t + u''(t)\frac{\Delta t^2}{2!} + u'''(t)\frac{\Delta t^3}{3!} + \ldots$$

- Thus $u'(t)$ is computed:

$$u'(t) = \frac{u(t+\Delta t) - u(t)}{\Delta t} + O(\Delta t^2)$$

Finite Difference Approximation (2)

The approximation is obtained by replacing a **differential operator** by a **finite difference**

$$u'(t) = \frac{u(t+\Delta t) - u(t)}{\Delta t}$$

- Substituting this in $u'(t) = f(t,u)$ gives

$$u(t+\Delta t) = u(t) + \Delta t\ f(t, u(t))$$

- If $t_0 = 0, t_{k+1} = t_k + \Delta t = \ldots = (k+1)\Delta t, u(t_k) = u_k$
- We thus get the **Explicit (forward) Euler** difference equation $u_{k+1} = u_k + \Delta t\ f(t_k, u_k)$

Explicit Euler: Alternative (easier) Formulation

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- Considering the general first order differential equation $x'(t) = f(t, x(t))$ with some initial condition $x(0) = x_0$
- Euler's (explicit) method based on

$$x'(t) = \lim_{h \Rightarrow 0} \frac{x(t+h) - x(t)}{h}$$

- Instead of letting, $h \Rightarrow 0$ take a finite $h > 0$ and

$$x'(t) \approx \frac{x(t+h) - x(t)}{h}$$

Explicit Euler: Alternative (easier) Formulation (2)

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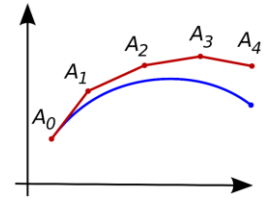
- Thus Euler's Explicit Method becomes

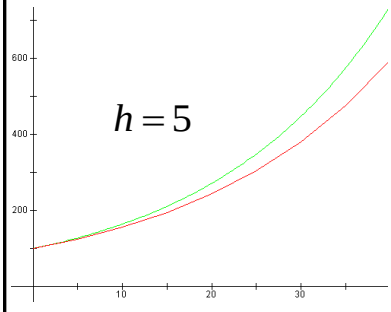
$$x(t+h) \approx x(t) + hx'(t) = x(t) + hf(t, x(t))$$

- Which is:
  - Simple to program
  - Very inefficient
  - It sometimes gives totally erroneous results
  - Highly dependent on the "right" choice for ***h***
  - Error is proportional in the first order with the step-size ***h*** → Euler is a "**first order method**"



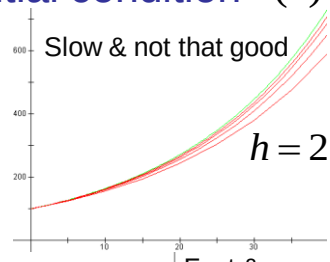
Euler's Method - Example

- Let us apply Euler's method to the equation $x'(t) = 0.05 \cdot x$ which has as solution $x = 100 \cdot e^{0.05t}$
- Considering the initial condition $x(0) = 100$



$h = 5$

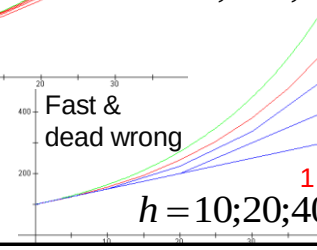
Green is the exact solution
Red is Euler's Method



Slow & not that good

48 Steps

$h = 2.5; 1.25; 0.625$



Fast &
dead wrong

1 Step

$h = 10; 20; 40$

Implicit Euler's method

- Instead of using the value of the derivative at the present point in time ***t***, use the value of the derivative at the future point in time ***t+h***:

$$x'(t) = \lim_{h \Rightarrow 0} \frac{x(t) - x(t-h)}{h}$$

- Again, with a finite h we get an approximate equation

$$x'(t) \approx \frac{x(t) - x(t-h)}{h}$$

- And thus

$$x(t) \approx x(t-h) + hx'(t) = x(t-h) + hf(t, x(t))$$

Implicit Euler's method (2)

- As can be seen in
$$x(t) \approx x(t-h) + hx'(t) = x(t-h) + hf(t, x(t))$$
- The unknown value ***x(t)*** appears on **both sides** of the equation, and as an argument for the function ***f(t,x)*** **on the right hand side**.
- This method is known as the **Implicit Euler method**.
- Finding ***x(t)*** requires solving (possibly numerically) the equation for ***x(t)***
- However, if an analytic formula for ***x(t)*** exists, the method is very easy to use
- To solve Implicit Euler you need an **iterative solver**

Stability of Implicit Euler

- Considering $f(t, x) = -\lambda x$
$$x_{k+1} = x_k - \lambda h x_{k+1} \Leftrightarrow (1+h)x_{k+1} = x_k$$
- And therefore
$$x_{k+1} = \left(\frac{1}{1+\lambda h}\right) \quad x_k = \left(\frac{1}{1+\lambda h}\right)^k x_0$$
- If $\lambda > 0$ which is the condition for a stable equation, we find that $x_k \to 0$ for all values of λ and ***t***.
- This method is called **unconditionally stable**
- The main advantage of an implicit method over an explicit one is clearly the stability

Stability of Implicit Euler (2)

- It is possible to take **larger time steps** without worrying about unphysical behavior
- Large time steps
  - Can make convergence to the steady state slower
  - But at least there will be no divergence
- Drawback – implicit methods are more complicated
  - Can involve nonlinear systems of equations to be solved in every time step

Other Methods – Runge-Kutta

- A slightly more complicated method for the solution of the generic first order differential equation $x'(t) = f(t, x(t))'$ is the Runge-Kutta method
- A fundamental theorem of calculus reads

$$x(t_j + h) - x(t_j) = \int_{t_j}^{t_j+h} x'(\tau)d\tau = \int_{t_j}^{t_j+h} f(\tau, x(\tau))d\tau$$

- An approximation for $x(t+h)$ is the approximation of the integral on the right hand side
- For numerical integration we apply the midpoint rule

$$\int_a^b g(\tau)d\tau \approx (b-a)g\left(\frac{a+b}{2}\right)$$

Other Methods – Runge-Kutta (2)

- First, this approximation leads to the following formula

$$x(t_j + h) \approx x(t_j) + hf\left(t_j + \tfrac{h}{2}, x(t_j + \tfrac{h}{2})\right)$$

- There is a big problem however:
  - We do not know the value of $x(t+h)$ at the midpoint $t_j + \frac{h}{2}$
- We must use an approximation, and we choose Euler's explicit method for this

$$x(t_j + \tfrac{h}{2}) \approx x(t_j) + \tfrac{h}{2} f(t_j, x(t_j))$$

- The final form for the new method thus reads

$$x(t_j + h) \approx x(t_j) + hf\left(t_j + \tfrac{h}{2}, x(t_j) + \tfrac{h}{2} f(t_j, x(t_j))\right)$$

Classical Predator-Prey Model

- Two species system:
  - Predators **P**
  - Preys **V**
- Predators are the only factor cutting down the prey population
- The remaining prey population breeds without limitations
- Predators' breeding rate is proportional to their catch

Classical Predator-Prey Model (2)

- The number of predators is limited by death rate

$$V' = kV - aVP$$
$$P' = bVP - dP$$

Also known as Lotka–Volterra equations

- Where:
  - ***k*** is the birth rate for prey
  - ***a*** is catch rate
  - ***b*** characterizes the efficiency with which predators use their catch to produce more predators
  - ***d*** is the death rate for predators

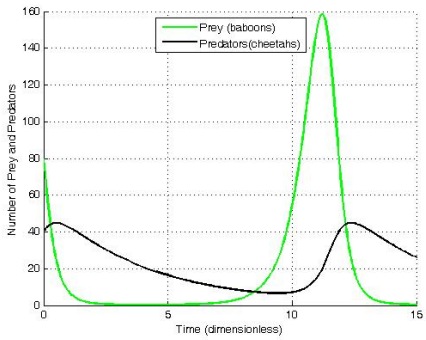
Classical Predator-Prey Model (3)

- The non-trivial equilibrium of the system

$$\begin{cases} kv - aVP = 0 \\ bVP - dP = 0 \end{cases} \Rightarrow \begin{cases} P = \frac{k}{a} = P_{eq} \\ V = \frac{d}{b} = V_{eq} \end{cases}$$

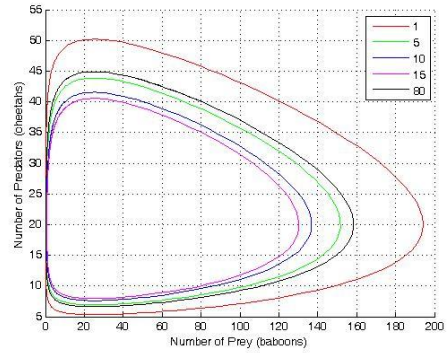
- Note the dependence on parameters at the equilibrium
- The lines $P = P_{eq}$ and $V = V_{eq}$ divide the first quadrant into four parts with different signs for the derivatives P' and V'

Predator-Prey Model Examples



- Problem at the lower limit of the prey population

- The solution is in a state of dynamic equilibrium – inside of the ellipses



Systems of Differential Equations

- Systems of differential equations describe the dynamics of complicated models
- There are usually two or more state variables $x_j(t)$ whose time development should be studied
  - For a specified time interval
  - For an arbitrary long period of time
- Some systems contain both **algebraic** and **differential equations** (DAEs)
- Two-dimensional models are easy to analyze
  - It is often possible to draw pictures of what is going on

Systems of Differential Equations (2)

- Generic form of a system of differential equations

$$x_1'(t) = f_1(t, x_1(t), x_2(t), \ldots, x_n(t))$$
$$x_2'(t) = f_2(t, x_1(t), x_2(t), \ldots, x_n(t))$$
$$\ldots$$
$$x_n'(t) = f_n(t, x_1(t), x_2(t), \ldots, x_n(t))$$

- If none of the functions f_j depend explicitly on t, the system is **autonomous**
- If every function f_j is linear, the system is said to be **linear**

Systems of Differential Equations (3)

- In order to have a unique solution
  - Initial and/or boundary conditions are needed
- Initial conditions are given at the moment $t = 0$
- Sometimes conditions are also given at the end point of the time interval
- It is also possible that part of the conditions are specified at the starting point and part at the end

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General Model Behavior

- Systems with two state variables can exhibit: equilibrium and limit cycles
- Equilibrium behavior:
  - **Stable**: starting near an equilibrium, will keep you near that equilibrium
  - **Asymptotically stable**: starting near an equilibrium, will drift you closer and closer to the equilibrium
  - **Unstable**: starting exactly at the equilibrium, will keep you there. Any perturbation, however small, will drive you away
  - **Saddle point**: depending on the direction w.r.t. the equilibrium you can either drift towards it or away from it

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General Model Behavior (2)

- Limit cycles:
  - **Neutral**: small perturbations will move you to another cycle
  - **Stable**: the effect of small perturbations will gradually disappear and the system drifts back to the original cycle
  - **Unstable**: small perturbations drive the system away from the cycle
- Possibly only numerical results
- Usually the long-term behavior is what matters

Table of Contents

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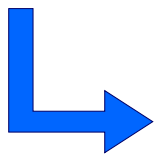
- Mathematical Modeling
- **Numerical Methods used in HPSC**
  - Systems of Differential Equations: ODEs & PDEs
  - **Automatic Differentiation**
  - Solving Optimization Problems
  - Solving Nonlinear Equations
  - Basic Linear Algebra, Eigenvalues and Eigenvectors
  - Chaotic systems
- HPSC Program Development/Enhancement: from Prototype to Production
- Visualization, Debugging, Profiling, Performance Analysis & Optimization

Automatic Differentiation – Motivation

- ***Design optimization***
- ***Sensitivity analysis & Parameter identification***
- ***Data assimilation problems***
- ***Inverse problems (data assimilation)***
- ***Solving ODE, PDE, DAE, …***
- ***Linear approximation & Curve fitting***

Derivative information required



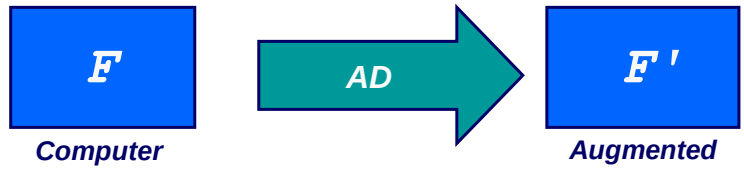
Numeric Differentiation

Symbolic Differentiation

Automatic Differentiation

Automatic Differentiation (AD)

- Semantic transformation:
  - Given a computer code **F**, AD generates a new program **F'** which applies the chain rule of differential calculus to elementary operations for which the derivatives are known

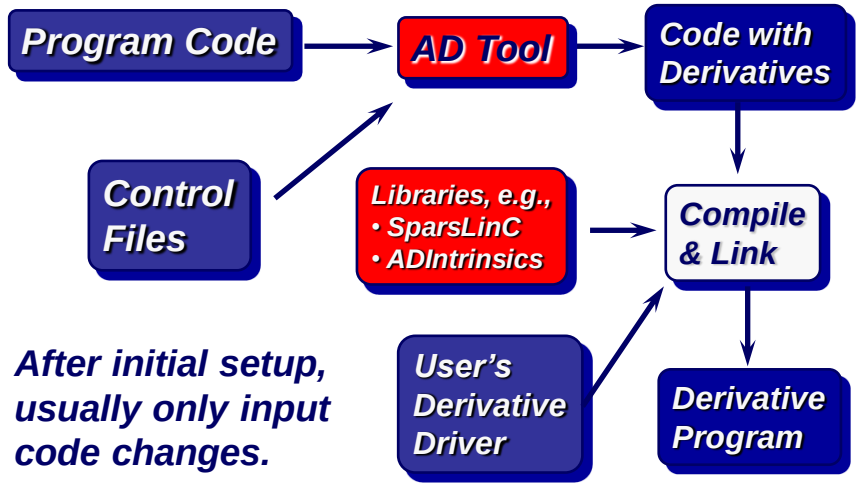


Computer Program — *Augmented Computer Program*

AD Advantages

- Generates truncation- and cancellation error-free derivatives
- Generates a program for the computation of derivative values, not of derivative formulae
- The associativity of the chain rule allows for a wide range of choices in accumulating derivatives → forward & reverse modes and generalizations

The AD Process



After initial setup, usually only input code changes.

AD-Tool Implementations

- Source Transformation (ST)
  - Compiler-based technique → generate new code that **explicitly** computes derivatives
  - **Advantages**: entire context known at compile-time → efficient code, transparency
  - **Drawback**: difficult implementation
- Operator Overloading (OO)
  - Extends elementary operations & functions to also **implicitly** compute derivatives
  - **Requires**: redeclaration of active variables to the new overloaded types
  - **Advantages**: easy implementation & „same" source code
  - **Drawback**: granularity → inefficient code

Some AD Tools

http://www.autodiff.org

Fortran 77, some Fortran 90:

- ADIFOR 3.0/ADJIFOR (RM, ∂f , $\partial^2 f$): Alan Carle & Mike Fagan (Rice)
- Tapenade (RM, ∂f): Laurent Hascoet (INRIA)
- TAMC/TAF (RM, ∂f): Ralf Giering (FastOpt GmbH).

ANSI-C/C++:

- ADOL-C: (FM/RM, $\partial^k f$): Andreas Griewank & Co. (TU Dresden)
- ADIC: (FM/RM, $\partial^k f$): Hovland (ANL)

Application Specific:

- Cosy-Infinity (Remainder Differential Algebra): Martin Berz (U Michigan)
- TOMLAB/MAD (AD of Matlab): Shaun Forth (RMCS Shrivenham)
- ADiMat (AD of Matlab): Andre Vehreschild (RWTH Aachen)

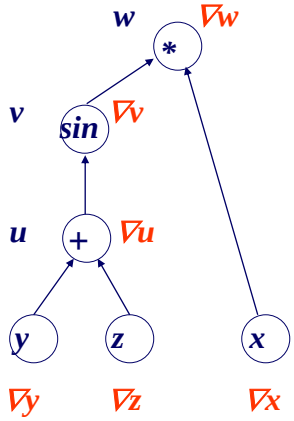
OpenAD/F:

- AD Framework: J. Utke & U. Naumann (ANL & RWTH Aachen)

Forward Mode - FM

Example code f: $w = x * \sin(y+z)$

Original code and derivative statements:



$\nabla u = \nabla y + \nabla z$

$u = y + z$

$\nabla v = \cos(u) * \nabla u$

$v = \sin(u)$

$\nabla w = \nabla v * x + v * \nabla x$

$w = v * x$

If $(\nabla x, \nabla y, \nabla z) = (1, 0, 0)$

$\rightarrow \nabla w$ ***computes*** $\partial w / \partial x$

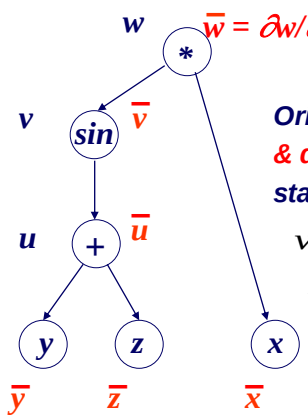
Each variable t ***is associated with a derivative object*** ∇t

Forward Mode Facts

- Computes $\partial f / \partial t$*S (S is called "seed matrix" – $[\nabla x, \nabla y, \nabla z]$) by propagating sensitivities of *intermediate values* with respect to *input values*
- For *p* input values of interest, ***runtime*** and ***memory*** scale approximately with *p*. May be much less e.g. for **sparse Jacobians**
- FM is appropriate for moderate *p*'s

Reverse Mode - RM

The same example code f: w = x * sin(y+z)



Original code & derivative statements:

$$v_k = f_k(\ldots, v_j, \ldots)$$

$$\bar{v}_j = \bar{v}_k \cdot \sum_k \frac{\partial f_k}{\partial v_j}$$

```
u = y + z
v = sin(u)
w = v * x
x̄ += w̄ * v
v̄ += w̄ * x
ū += v̄*cos(u)
z̄ += ū
ȳ += ū
```

If $\bar{w} = 1 \rightarrow (\bar{x}, \bar{y}, \bar{z})$ contains

$\nabla w = (\partial w/\partial x, \partial w/\partial y, \partial w/\partial z)$

Each variable t is associated with an adjoint object $\bar{t}$, the differentiated expressions are accumulated in the reverse order

Reverse Mode Facts

- Computes $W^T * \partial f / \partial t$ by propagating sensitivities of *output values* with respect to *intermediate values*
- For q output values of interest, the ***runtime*** scales with q. ***Memory requirements*** are harder to predict → greatly depend on the structure & implementation of program/AD-tool
- RM is great for computing „**long gradients**“ – small q‘s and big p‘s

Forward & Reverse Mode Example

given function $f(x, y, z) = (xy + \cos z)(x^2 + 2y^2 + 3z^2)$, the partial derivatives are

$$\frac{\partial f}{\partial x} = y \cdot (x^2 + 2y^2 + 3z^2) + (xy + \cos z) \cdot 2x = 3x^2 y + 2y^3 + 3yz^2 + 2x \cos z,$$

$$\frac{\partial f}{\partial y} = x \cdot (x^2 + 2y^2 + 3z^2) + (xy + \cos z) \cdot 4y = x^3 + 6xy^2 + 3xz^2 + 4y \cos z,$$

$$\frac{\partial f}{\partial z} = -\sin z \cdot (x^2 + 2y^2 + 3z^2) + (xy + \cos z) \cdot 6z$$

$$= -x^2 \sin z - 2y^2 \sin z - 3z^2 \sin z + 6xyz + 6z \cos z.$$

$$\nabla f = \left[\frac{\partial f}{\partial x} \quad \frac{\partial f}{\partial y} \quad \frac{\partial f}{\partial z} \right]^T$$

Forward Mode

Code list	+	Gradient entries
$u_1 = x,$		$\nabla u_1 = [1,0,0],$
$u_2 = y,$		$\nabla u_2 = [0,1,0],$
$u_3 = z,$		$\nabla u_3 = [0,0,1],$
$u_4 = u_1 u_2,$		$\nabla u_4 = u_1 \nabla u_2 + u_2 \nabla u_1 = [0,u_1,0] + [u_2,0,0] = [u_2,u_1,0],$
$u_5 = \cos u_3,$		$\nabla u_5 = (-\sin u_3)\nabla u_3 = [0,0,-\sin u_3],$
$u_6 = u_4 + u_5,$		$\nabla u_6 = \nabla u_4 + \nabla u_5 = [u_2,u_1,-\sin u_3],$
$u_7 = u_1^2,$		$\nabla u_7 = 2u_1 \nabla u_1 = [2u_1,0,0],$
$u_8 = 2u_2^2,$		$\nabla u_8 = 4u_2 \nabla u_2 = [0,4u_2,0],$
$u_9 = 3u_3^2,$		$\nabla u_9 = 6u_3 \nabla u_3 = [0,0,6u_3],$
$u_{10} = u_7 + u_8 + u_9,$		$\nabla u_{10} = \nabla u_7 + \nabla u_8 + \nabla u_9 = [2u_1,4u_2,6u_3],$
$u_{11} = u_6 u_{10},$		$\nabla u_{11} = u_6 \nabla u_{10} + u_{10} \nabla u_6 = [2u_6 u_1 + u_{10} u_2, 4u_6 u_2 + u_{10} u_1, 6u_6 u_3 - u_{10} \sin u_3].$

$$\nabla f(x,y,z) = \nabla u_{11} = [3x^2 y + 2x\cos z + 2y^3 + 3yz^2,\ 6xy^2 + 4y\cos z + x^3 + 3xz^2,\ 6xyz + 6z\cos z - x^2 \sin z - 2y^2 \sin z - 3z^2 \sin z].$$

Correct!

Reverse Mode

Code list	+	Adjoints
$u_1 = x,$		$\frac{\partial u_{11}}{\partial u_{11}} = 1,\ \frac{\partial u_{11}}{\partial u_{10}} = u_6,\ \frac{\partial u_{11}}{\partial u_9} = \frac{\partial u_{11}}{\partial u_{10}}\frac{\partial u_{10}}{\partial u_9} = u_6,$
$u_2 = y,$		$\frac{\partial u_{11}}{\partial u_8} = \frac{\partial u_{11}}{\partial u_{10}}\frac{\partial u_{10}}{\partial u_8} = u_6,\ \frac{\partial u_{11}}{\partial u_7} = \frac{\partial u_{11}}{\partial u_{10}}\frac{\partial u_{10}}{\partial u_7} = u_6,$
$u_3 = z,$		$\frac{\partial u_{11}}{\partial u_6} = u_{10},\ \frac{\partial u_{11}}{\partial u_5} = \frac{\partial u_{11}}{\partial u_6}\frac{\partial u_6}{\partial u_5} = u_{10},\ \frac{\partial u_{11}}{\partial u_4} = \frac{\partial u_{11}}{\partial u_6}\frac{\partial u_6}{\partial u_4} = u_{10},$
$u_4 = u_1 u_2,$		$\frac{\partial u_{11}}{\partial u_3} = \frac{\partial u_{11}}{\partial u_9}\frac{\partial u_9}{\partial u_3} + \frac{\partial u_{11}}{\partial u_5}\frac{\partial u_5}{\partial u_3} = 6u_6 u_3 - u_{10}\sin u_3,$
$u_5 = \cos u_3,$		$\frac{\partial u_{11}}{\partial u_2} = \frac{\partial u_{11}}{\partial u_4}\frac{\partial u_4}{\partial u_2} + \frac{\partial u_{11}}{\partial u_8}\frac{\partial u_8}{\partial u_2} = u_{10}u_1 + 4u_6 u_2,$
$u_6 = u_4 + u_5,$		$\frac{\partial u_{11}}{\partial u_1} = \frac{\partial u_{11}}{\partial u_4}\frac{\partial u_4}{\partial u_1} + \frac{\partial u_{11}}{\partial u_7}\frac{\partial u_7}{\partial u_1} = u_{10}u_2 + 2u_6 u_1.$
$u_7 = u_1^2,$		
$u_8 = 2u_2^2,$		
$u_9 = 3u_3^2,$		
$u_{10} = u_7 + u_8 + u_9,$		
$u_{11} = u_6 u_{10},$		

$$\nabla f(x,y,z) = \left[\frac{\partial u_{11}}{\partial u_1}, \frac{\partial u_{11}}{\partial u_2}, \frac{\partial u_{11}}{\partial u_3}\right] = [3x^2 y + 2x\cos z + 2y^3 + 3yz^2,\ 6xy^2 + 4y\cos z + x^3 + 3xz^2,\ 6xyz + 6z\cos z - x^2 \sin z - 2y^2 \sin z - 3z^2 \sin z].$$

Correct!

Divided Differences

First order differentiation

Forward differentiation: $\frac{\partial f}{\partial x_m} = \frac{f(x_1,\ldots,x_m+h,\ldots,x_n) - f(x_1,\ldots,x_m,\ldots,x_n)}{h} + O(h)$

Backward differentiation: $\frac{\partial f}{\partial x_m} = \frac{f(x_1,\ldots,x_m,\ldots,x_n) - f(x_1,\ldots,x_m-h,\ldots,x_n)}{h} + O(h)$

Centered differentiation: $\frac{\partial f}{\partial x_m} = \frac{f(x_1,\ldots,x_m+h,\ldots,x_n) - f(x_1,\ldots,x_m-h,\ldots,x_n)}{2h} + O(h^2)$

Second order differentiation

$$\frac{\partial^2 f}{\partial x_m^2} = \frac{f(x_1,\ldots,x_m+h,\ldots,x_n) - 2f(x_1,\ldots,x_m,\ldots,x_n) + f(x_1,\ldots,x_m-h,\ldots,x_n)}{h^2} + O(h^2)$$

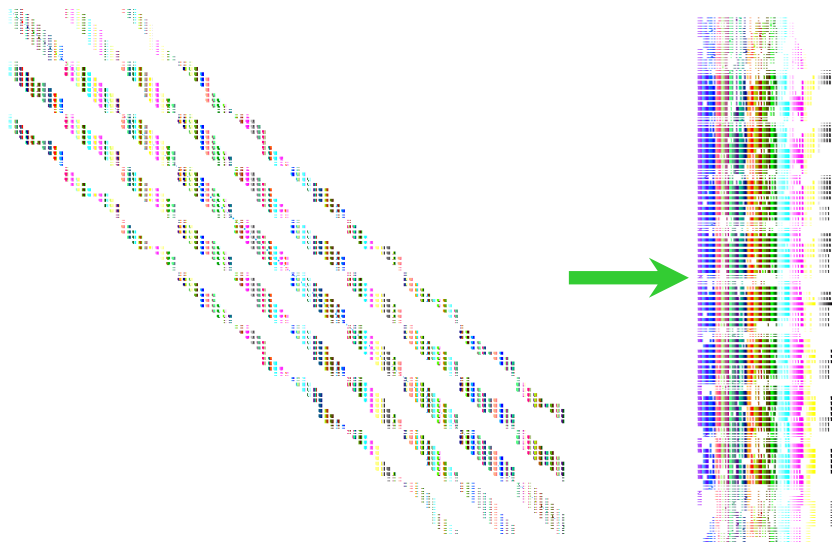
Which mode to use?

- Use **forward mode** when
  - # **independents** is very small
  - Only a directional derivative **Jv** is needed
  - Reverse mode is not tractable
- Use **reverse mode** when
  - # **dependents** is very small
  - Only $\mathbf{J^T v}$ is needed

Case Study – Matrix Coloring

- Jacobian matrices are often sparse
- The forward mode of AD computes J × S, where S is usually an identity matrix or a vector
- One can "**compress**" Jacobian by choosing S such that *structurally orthogonal* columns are combined
- A set of columns are structurally orthogonal if no two of them have nonzeros in the same row
- Equivalent problem: color the graph whose adjacency matrix is $J^T J$
- Equivalent problem: distance-2 color the bipartite graph of J

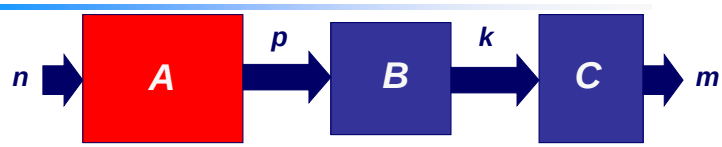
Compressed Jacobian



What is feasible & practical

- Key point:
  - Forward mode computes JS at cost proportional to number of columns in S
  - Reverse mode computes $J^T W$ at cost proportional to number of columns in W
- Jacobians of functions
  - Small number (1—1000) of **independent** variables (FM)
  - Small number (1—100) of **dependent** variables (RM)
- Extremely large, but (very) sparse Jacobians and Hessians
- Jacobian-vector products (forward mode)
- Transposed-Jacobian-vector products (adjoint mode)
- Hessian-vector products (forward + adjoint modes)

Scenarios

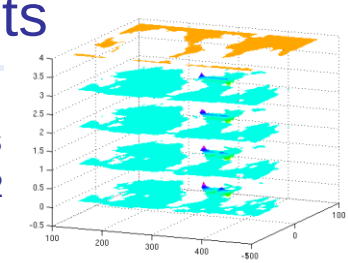


- n small: use FM on full computation
- m small: use RM on full computation
- m & n large, p small: use RM on A, FM on B&C
- m & n large, k small: use RM on A&B, FM on C
- n, p, k, m large, Jacobians of A, B, C sparse: compressed FM
- n, p, k, m large, Jacobians of A, B, C low rank: scarce FM
- n, p, k, m large: Jacobians of A, B, C dense: what to do?

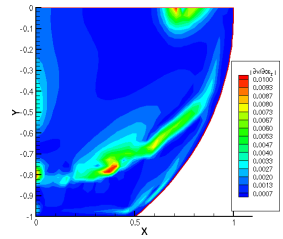
Issues with Black Box Differentiation

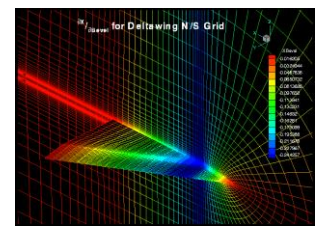
- Source code may not be available or may be difficult to work with
- Simulation may not be (chain rule) differentiable
  - Feedback due to adaptive algorithms
  - Non-differentiable functions
  - Noisy functions
  - Convergence rates
  - Etc.
- Accurate derivatives may not be needed – FD might be cheaper
- Differentiation and discretization do not commute

Application highlights

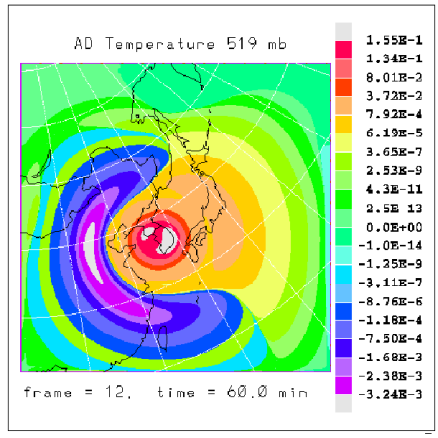


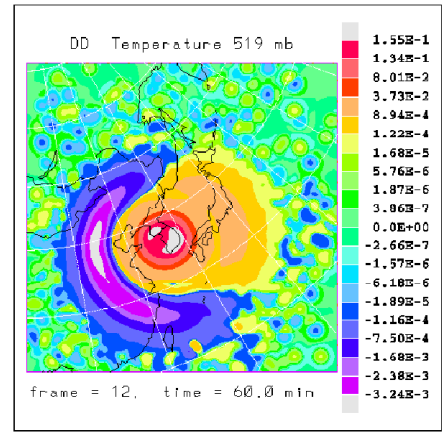
- Atmospheric chemistry
- Breast cancer biostatistical analysis
- CFD: CFL3D, NSC2KE, Fluent 4.52
- Chemical kinetics
- Climate and weather: MITGCM, MM5, CICE
- Semiconductor device simulation
- Water reservoir simulation





Sensitivity Analysis: Mesoscale Weather Modeling





AD Conclusions & Future Work

- Automatic differentiation research involves a wide range of combinatorial problems
- AD is a powerful tool for scientific computing
- Modern automatic differentiation tools are robust and produce efficient code for complex simulation codes
  - Requires an industrial-strength compiler infrastructure
  - Efficiency requires sophisticated compiler analysis
- Effective use of automatic differentiation depends on insight into problem structure
- Future Work
  - Further develop and test techniques for computing Jacobians that are effectively sparse or effectively low rank
  - Develop techniques to automatically generate complex and adaptive checkpointing strategies