Optical tomography reconstruction: inversion based on adjoint differentiation

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Overview of presentation

- General problem of inversion of complex simulations
- Introduction to optical tomography
- Propagation of IR photons in tissue, a diffusion process
- Simulation of diffusion process by finite-difference method - *"the forward problem"*
- Reconstruction of optical properties using adjoint differentiation - *"the inverse problem"*
- Examples of IR tomographic reconstructions
- Applications & more details about adjoint differentiation

Acknowledgements

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- General discussions
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Inversion of complex simulations

- There are BIG problems that
  - require complex numerical simulations to describe phenomena
  - are nonlinear in nature
  - one would like to fit to data, that is, solve the inverse problem
- Approximations are typically made in forward simulation to facilitate the solution of the inverse problem
  - perturbation methods (Born approximation)
  - truncated basis-function expansion
  - linearization of the problem
  - degradation of the spatial resolution
- Advanced methods are needed to invert large numerical simulations

Inversion of complex simulations

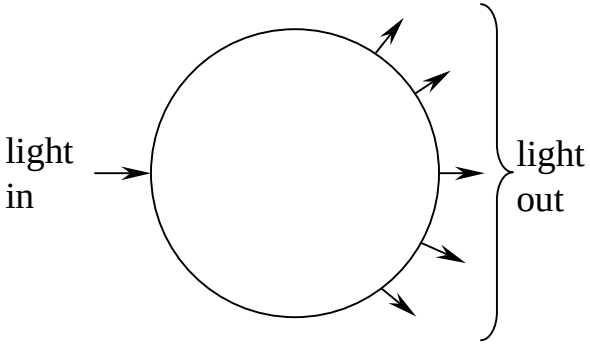
- Advanced techniques are required to cope with large data structures and numerous parameters
  - Optimization
    - gradient-based quasi-Newton methods (e.g., CG, BFGS)
    - adjoint differentiation for efficient calculation of gradients
    - multiscale methods for controlling optimization process
  - Bayesian methods
    - overcome ill posedness of inversion through use of prior knowledge
    - Markov chain Monte Carlo to characterize uncertainties
  - Appropriate higher-order models
    - Markov random fields
    - deformable geometrical models
    - but also consider lowest order, elemental representations

General uses of adjoint differentiation

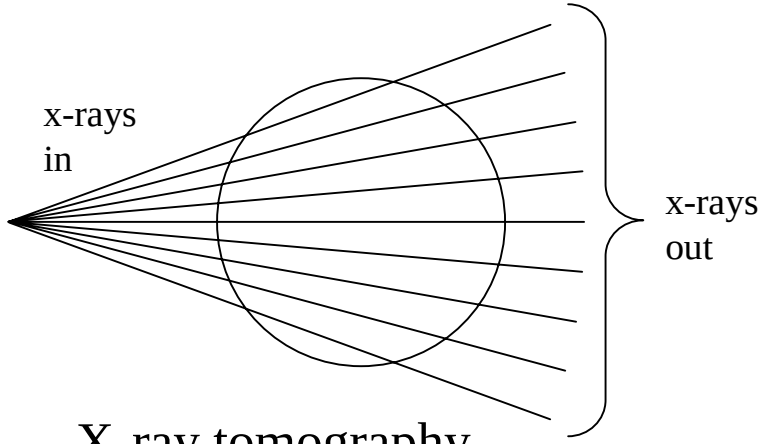
- Reconstruction: imaging through refractive media
  - seismology, medical and NDE ultrasound, ...
- Matching large-scale simulations to data:
  - atmosphere and ocean models, fluid dynamics, hydrodynamic
- Optimization in large engineering design problems:
  - optical lens systems, geometry of integrated circuits, aerodynamic shape, engines
- Uncertainty analysis
  - sensitivity of uncertainty variance to each contributing cause
- Markov Chain Monte Carlo
  - generation of random samples from a prob. dens. function

Optical tomography - general idea

- Shine light on tissue sample; measure light out



Optical tomography



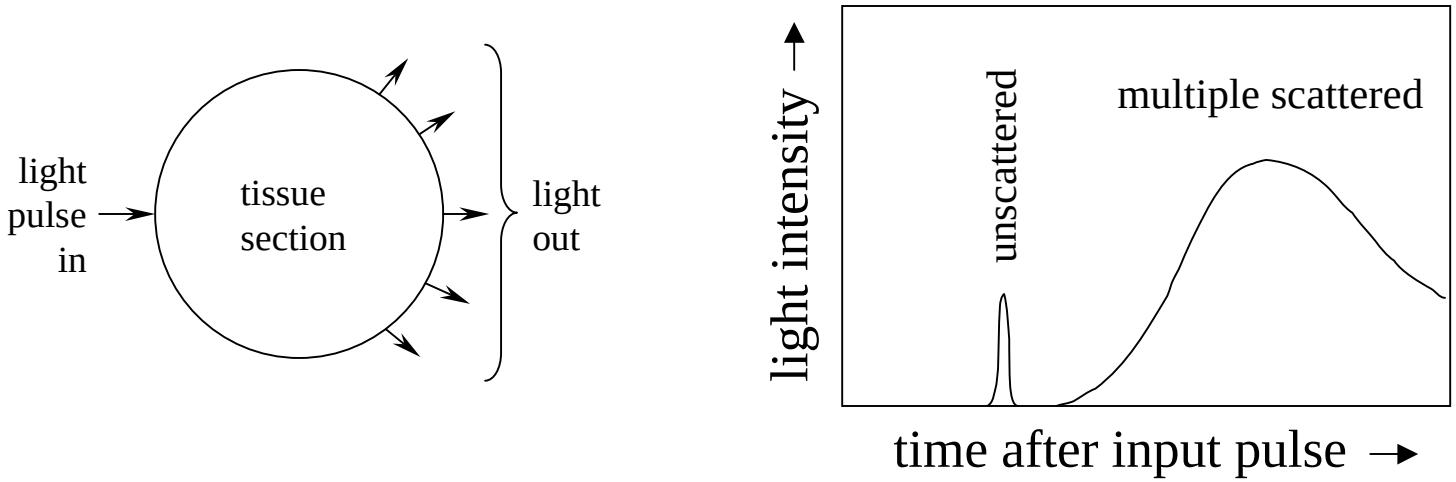
X-ray tomography

- Analogous to x-ray computed tomography, so:
  - Can one actually do optical tomography?
  - What are best operating conditions?
  - What are imaging properties and diagnostic uses?

Physics of propagation of light in tissue

- Basic processes are scattering and absorption of photons
  - absorption in tissue is minimal in *infrared* range
  - IR photons can actually pass through bone
  - for soft tissue, $\mu_{\text{scat}} \approx$ 1-10 cm^{-1}, $\mu_{abs} \approx 0.1\ \text{cm}^{-1}$
- Transport equation generally applies
- Diffusion equation often good approximation
  - valid when scattering is isotropic and without energy loss

Proposed experimental scheme

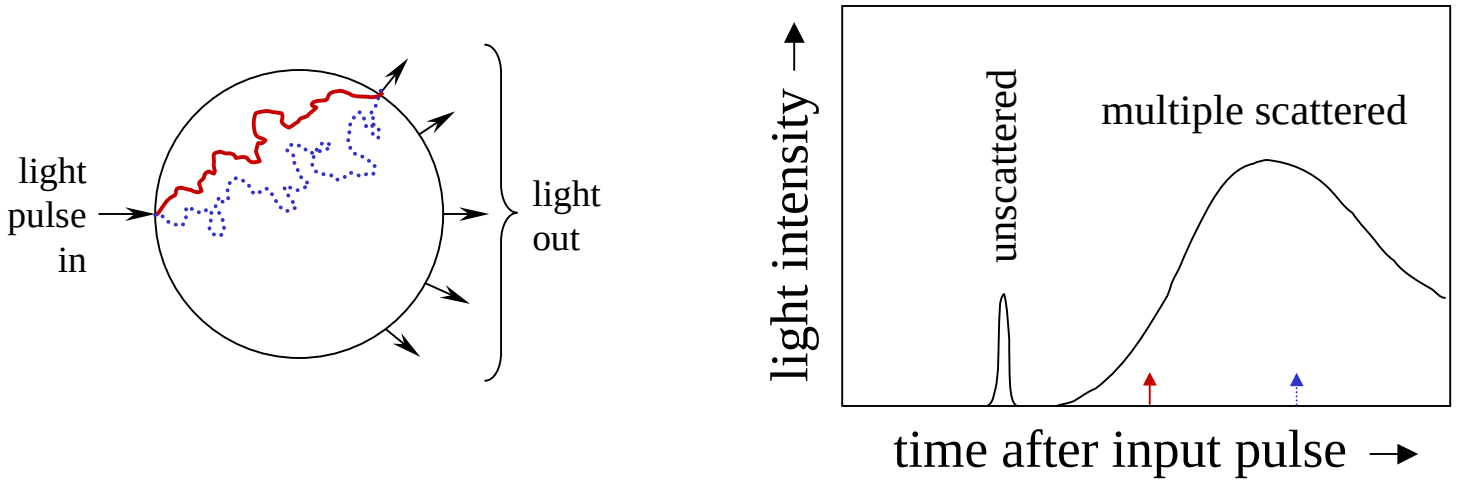


- Shine IR light pulse on tissue sample at several positions
- For each input pulse, measure at several output positions the light intensity vs. time with time resolution << 1 ns.
  - prompt, unscattered photons; few survive thick sections
  - multiply scattered photons; meander or diffuse through section

Alternative experimental schemes

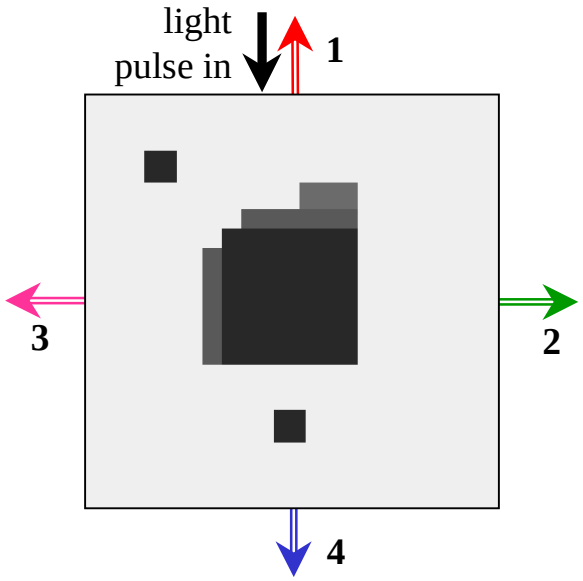
- Numerous types of measurements of the light transmitted through tissue sample are possible:
  - pulsed input; measure full time dependence distribution (delta-function response)
  - pulsed input; measure average time $< t >$ (first moment of time distribution)
  - modulated input; measure amplitude and phase of modulated output intensity (Fourier transform of delta-function response)
  - constant input; measure amplitude of output (integral of delta-function response)

Modeling of process

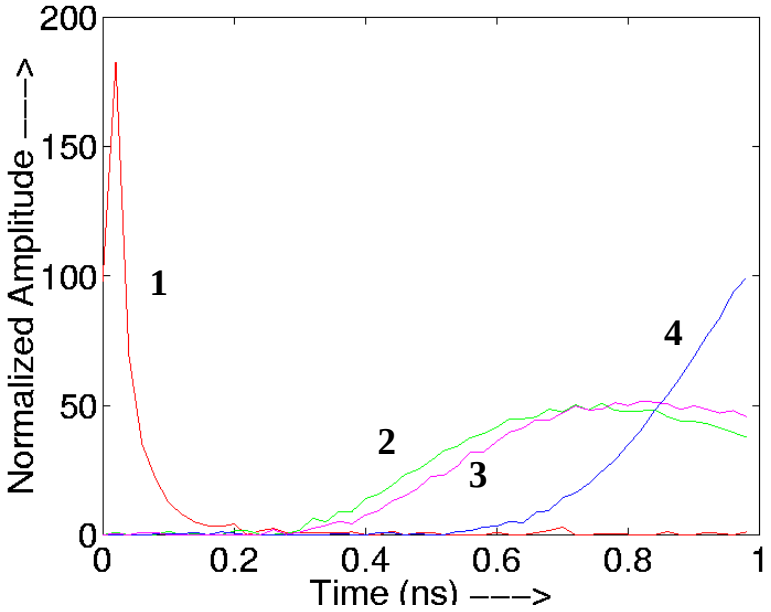


- IR light photons in broad, retarded peak literally "diffuse" by multiple scattering from source to detector
  - time is equivalent to distance traveled
  - diffusion equation models these multiply-scattered photons
  - these photons do not follow straight lines

Simulation of light diffusion in tissue



$0.7 < D < 1.4$ cm^{2}ns^{-1} (μ_a=0.1 cm^{-1})

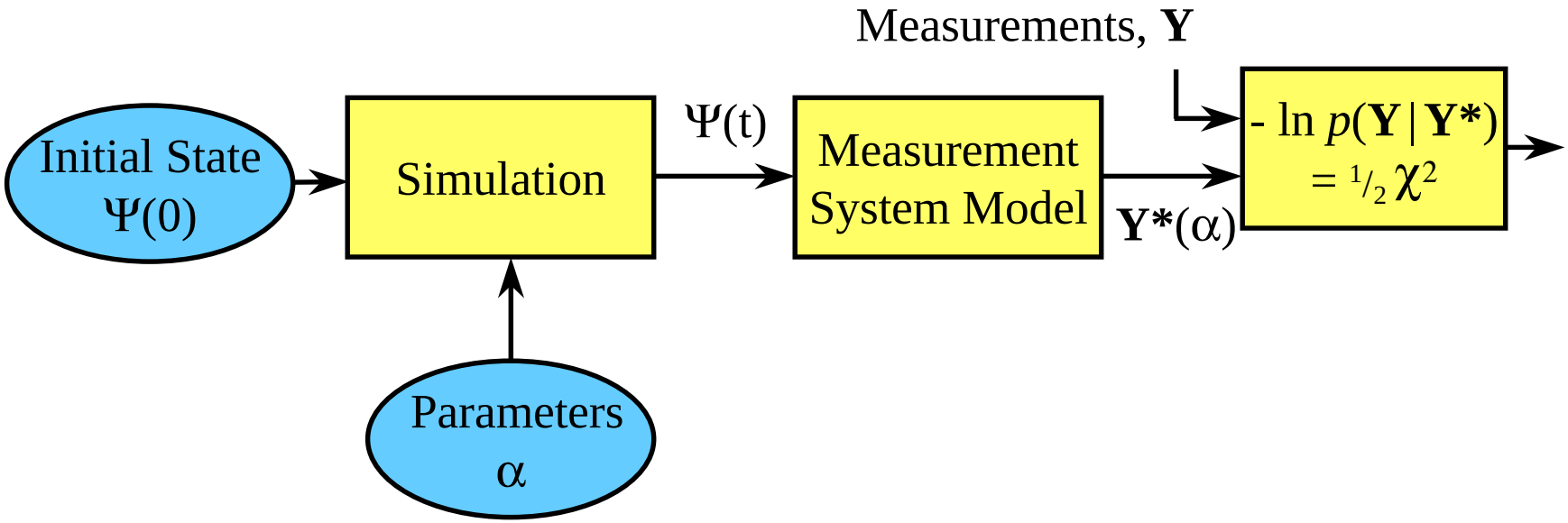


- for assumed distribution of diffusion coefficients (left)
- predict time-dependent output at four locations (right)
- reconstruction problem - determine image on left from data on right

Reconstruction problem

- Determine tissue properties from measurements
  - diffusion coefficient $D(x,y)$ and absorption coefficient $\mu_a(x,y)$, as a function of position - therefore, many unknowns
- Many problems must be overcome
  - photon paths depend on properties to be reconstructed
  - hence, inverse problem is nonlinear and difficult
  - measurements can only be calculated numerically; no analytic expression for measurements in terms of D and μ_a
  - gradients are desired for speedy gradient-based optimization
    - analytic gradients are not available
    - numerical gradients by perturbation too time consuming
    - **adjoint differentiation** crucial to success

Parameter estimation by fitting data



- Diagram describes general approach (analytical and computational)
- Find parameters (vector α) that minimize -ln *p*(**Y**| **Y***(α))
- Result is **maximum likelihood estimate** for α
  - also known as minimum-chi-squared or least-squares solution
- Optimization process is accelerated by using **gradient-based algorithms**; therefore need gradients of simulation and measurement processes

Diffusion equation

- Infrared light diffuses through tissue and bone
- Partial differential equation describes diffusion process
  - *U(x,y,t)* is intensity of diffused light (no angular dependence)

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left[D\frac{\partial U}{\partial x}\right] + \frac{\partial}{\partial y}\left[D\frac{\partial U}{\partial y}\right] - c\mu_{abs}U + S$$

  - where *D(x,y)* is position-dependent diffusion coefficient,
    $\mu_{abs}(x,y)$ is the linear absorption coefficient,
    c is the speed of light,
    S(x,y,t) is a source term;

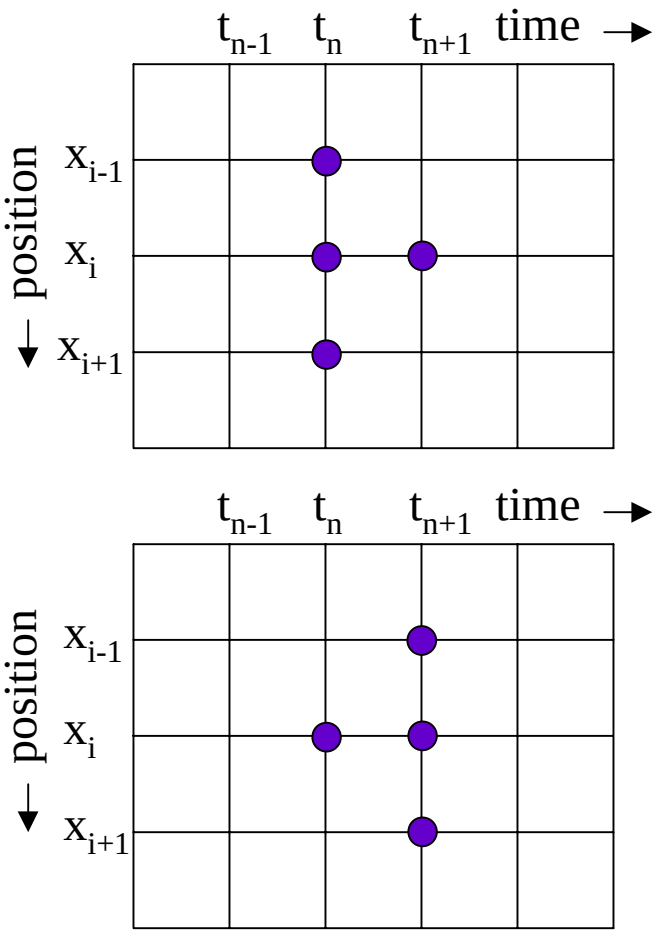
$D = c[3(\mu_{abs} + \mu'_{scat})]^{-1}$ (μ'_{scat} = effective scattering coefficient)

Method of finite differences

- Approximate derivatives by finite differences
  - wrt time: $\frac{\partial U}{\partial t} \Rightarrow \frac{\Delta U}{\Delta t} = \frac{U_{i,n+1} - U_{i,n}}{\Delta t}$
  - wrt position: $\frac{\partial^2 U}{\partial x^2} \Rightarrow \frac{U_{i+1,n} - 2U_{i,n} + U_{i-1,n}}{(\Delta x)^2}$
- Differential equation then leads to a set of linear equations to be solved to obtain time-step update
  - calculate time evolution, starting with initial conditions
- Question: at what time should second derivative wrt position be calculated, *n* or *n+1*?

Calculation of finite differences

- For diffusion equation, need
  - temporal first order derivative
  - spatial second order derivative
- Explicit technique
  - for step from time *n* to *n+1*, evaluate spatial derivative at *n*
  - **unstable** for moderate time steps
- Implicit technique
  - for step from time *n* to *n+1*, evaluate spatial derivative at *n+1*
  - inherently **stable**



Explicit method

- Evaluating position derivatives at *n*

$$\frac{U_{i,n+1} - U_{i,n}}{\Delta t} = D_i \frac{U_{i+1,n} - 2U_{i,n} + U_{i-1,n}}{(\Delta x)^2} - c\mu_i U_{i,n} + S_{i,n}$$

  - for clarity, ignore position dependence of *D* and *y* coord.
  - yields set of linear equations:

$$\boxed{\mathbf{U}_{n+1} = \mathbf{B}\mathbf{U}_n + b\mathbf{S}_n} \quad (b \text{ is a scalar constant})$$

- $\mathbf{U}_{n+1}$ at new time *n+1* is given **explicitly** in terms of state at previous $\mathbf{U}_n$
- Easy to calculate time steps (just matrix multiplication)
- Unfortunately, inherently **unstable** for moderate Δt

Implicit method

- Evaluating position derivatives at time *n+1*

$$\frac{U_{i,n+1} - U_{i,n}}{\Delta t} = D_i \frac{U_{i+1,n+1} - 2U_{i,n+1} + U_{i-1,n+1}}{(\Delta x)^2} - c\mu_i U_{i,n+1} + \tfrac{1}{2}(S_{i,n+1} + S_{i,n})$$

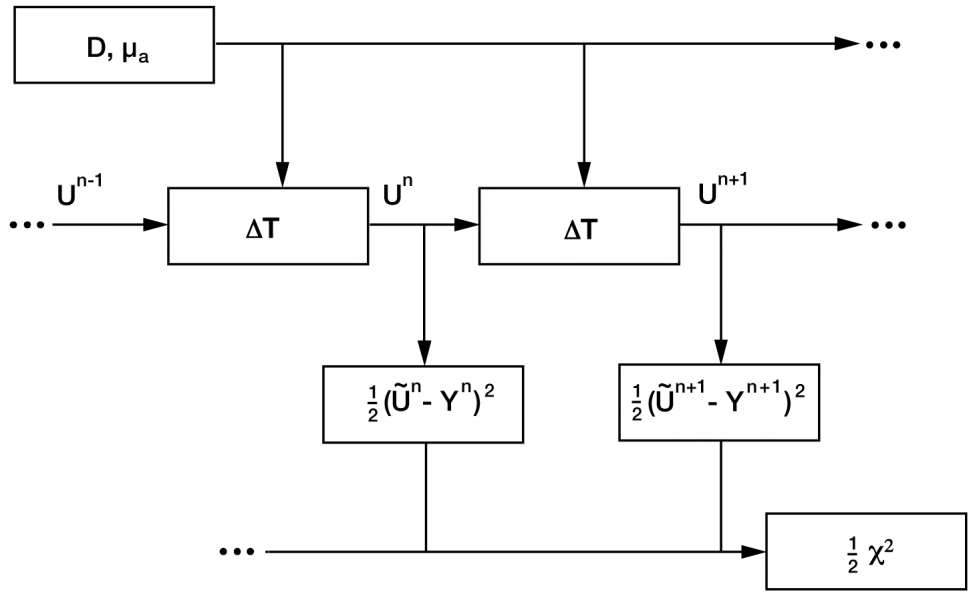
  - for clarity, ignore position dependence of *D* and *y* coord.
  - yields set of linear equations:

$$\boxed{\mathbf{A}\mathbf{U}_{n+1} = \mathbf{U}_n + a\,\mathbf{S}_n}$$ (*a* is a scalar constant)

- $\mathbf{U}_{n+1}$ at new time *n+1* is given **implicitly** in terms of state at previous time $\mathbf{U}_n$
- Must solve set of linear eqs. to calculate time steps
- Inherently **stable** for moderate Δt

Finite-difference calculation

- Data-flow diagram shows calculation of time-dependent measurements by finite-difference simulation
- Calculation marches through time steps Δt
  - new state $\mathbf{U}_{n+1}$ depends only on previous state $\mathbf{U}_n$



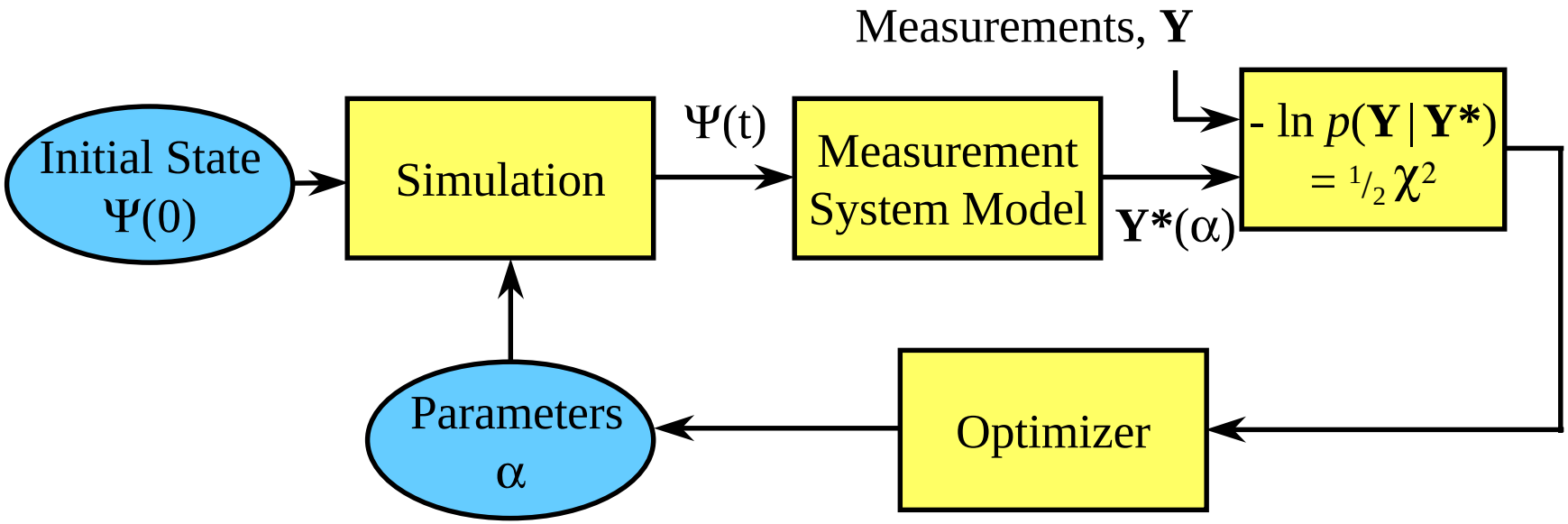
Inversion of forward calculation

- To find parameters $\alpha = (D, \mu_a)$, minimize minus-log-likelihood of data:

$$\phi(\alpha) = -\ln p(\mathbf{Y} \mid \alpha) = \tfrac{1}{2} \sum_m \frac{(Y_m - Y_m{}^*)^2}{\sigma_m^2} = \tfrac{1}{2} \chi^2$$

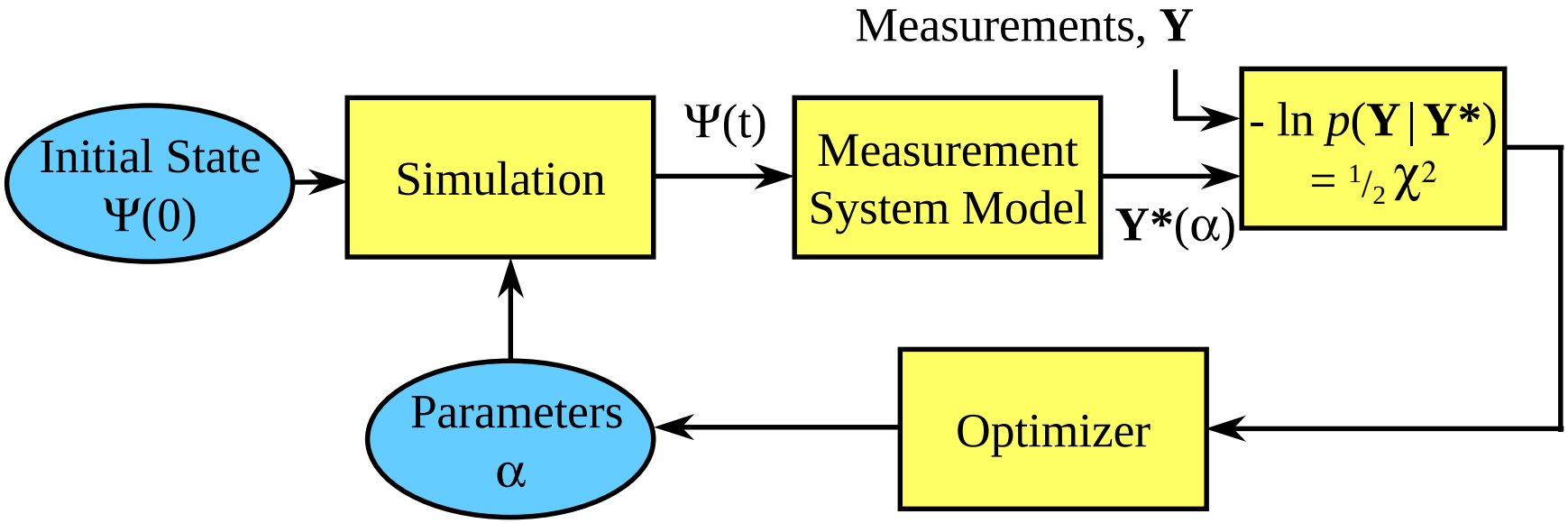
  - where Y_m is the mth measurement,
    $Y_m{}^*$ its predicted value (= $U_{s,n}$ at appropriate s and n),
    σ_m is rms noise in measurement
  - measurements are at fixed position, but at all times
- Problems for inverting diffusion process
  - inversion may be ill posed, a theoretical issue
  - have only numerical solution of forward simulation, so calculation of gradient poses practical problem

Parameter estimation by fitting data



- Find parameters (vector α) that minimize -ln $p(\mathbf{Y}|\ \mathbf{Y}^*(\alpha))$
- Result is **maximum likelihood estimate** for α
  - also known as minimum-chi-squared or least-squares solution
- Prior information can be used to overcome ill-posedness
- Bayesian approach

Maximum likelihood estimation by optimzation



- Find minimum in -ln $p(\mathbf{Y}|\ \mathbf{Y}^*(\alpha)) = \frac{1}{2}\chi^2$ by iteration over parameters α
- Optimization process is accelerated by using **gradient-based algorithms**; therefore need gradients of simulation and measurement processes
- **Adjoint differentiation** facilitates efficient calculation of gradients, i.e. derivative of scalar output ($\frac{1}{2}\chi^2$) wrt parameters α

Derivative calculation by finite differences

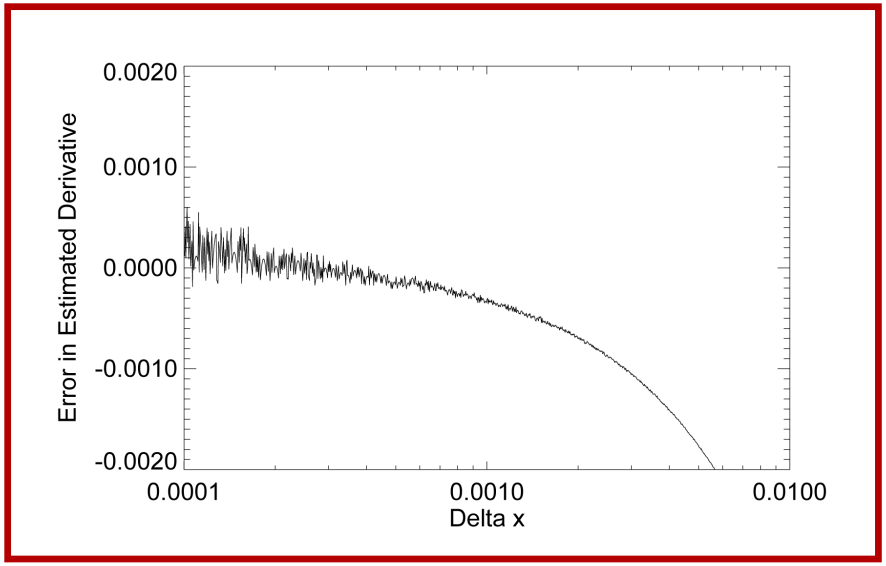
- Derivative for function defined as limit of ratio of finite differences:

$$\left.\frac{df}{dx}\right|_{x1} = \lim_{\Delta x \to 0} \frac{f(x1+\Delta x) - f(x1)}{\Delta x}$$

  Wish to estimate derivatives of calculated function for which there is no analytic relation between outputs and inputs

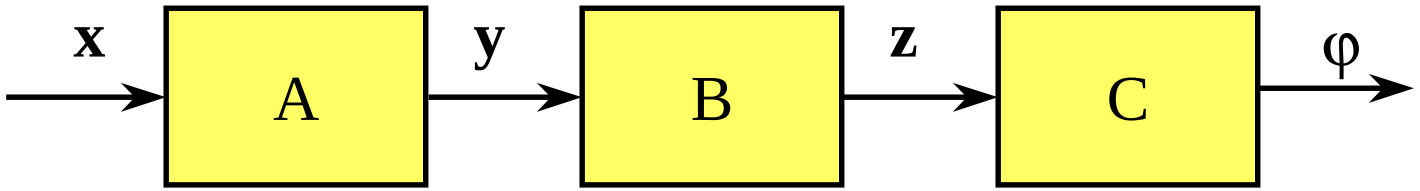
- Numerical estimation based on finite differences is problematical:
  - difficult to choose perturbation Δx
  - # function evaluation ~ # variables

- Estimation based on functionality implied by computer code is more reliable



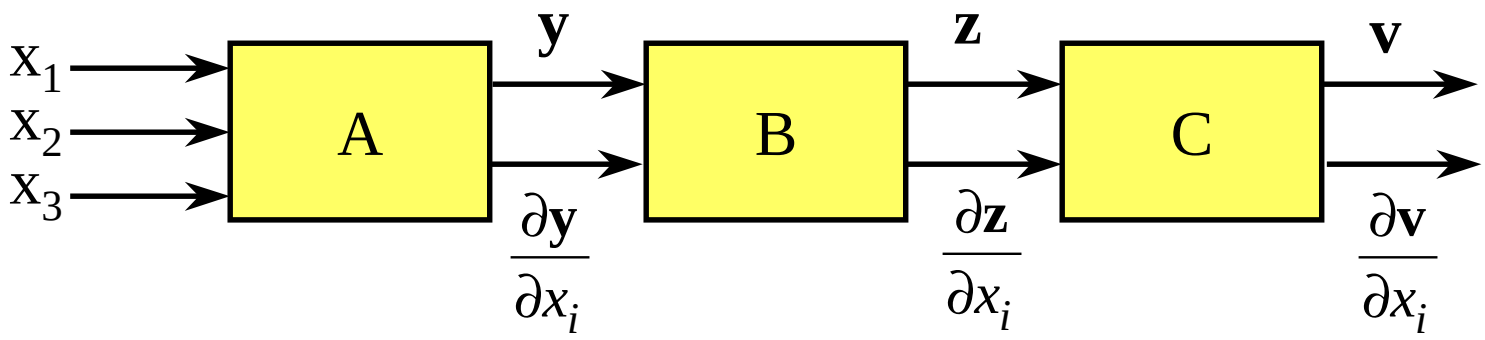
Error in derivative of sin(x) vs. Δx at $x = \pi/4$

Differentiation of sequence of transformations



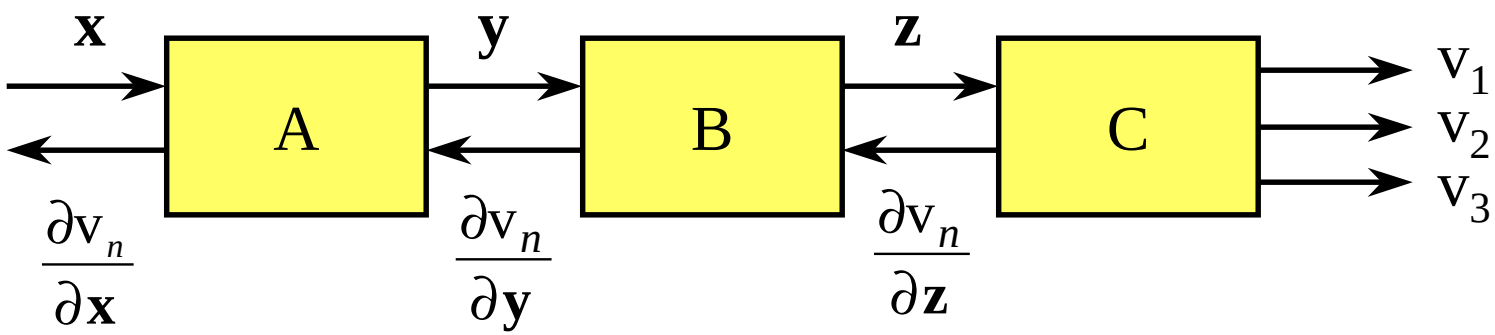
- Data-flow diagram shows sequence of transformations A->B->C that converts data structures **x** to **y** to **z** and to scalar φ (**forward calculation**)
- Desire derivatives of φ wrt all components of **x**, *assuming* φ is *differentiable*
- Chain rule applies: $$\frac{\partial \varphi}{\partial x_i} = \sum_{j,k} \frac{\partial y_j}{\partial x_i} \frac{\partial z_k}{\partial y_j} \frac{\partial \varphi}{\partial z_k}$$
- Two choices for summation order:
  - doing *j* before *k* means derivatives follow data flow (forward calculation)
  - doing *k* before *j* means derivatives flow in reverse (adjoint) direction

Derivatives for few variables in, many out



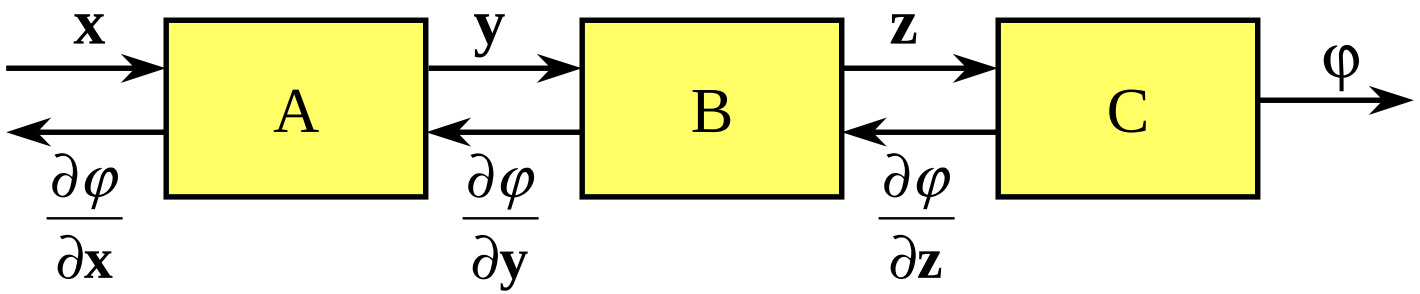
- Derivatives of a few input variables wrt many output variables
- Most efficient approach is to propagate derivatives wrt input variables in direction of forward calculation
- For *m* inputs:
  - computation takes about *m* times longer than forward calculation
  - intermediate storage required is *m* times larger than for forward calculation
- One obtains derivatives of all variables in forward calculation wrt each input

Derivatives for many variables in, few out



- Derivatives of many outputs wrt just a few output variables
- Most efficient approach is to propagate derivatives wrt output variables in reverse direction (also called **adjoint direction**)
- For *n* outputs:
  - computation takes on order of *n* times longer than forward calculation
  - intermediate storage required is *n* times larger than for forward calculation
- One obtains derivatives of each output variable wrt all variables in forward calculation

Adjoint Differentiation In Code Technique ADICT



- For sequence of transformations that converts data structure **x** to scalar φ
- Derivatives $\frac{\partial \varphi}{\partial \mathbf{x}}$ are efficiently calculated in the reverse (adjoint) direction
- **Code-based approach**: logic of adjoint code is based explicitly on the forward code or on derivatives of the forward algorithm
- **Not** based on the theoretical eqs., which forward calc. only approximates
- Only assumption is that φ is a **differentiable function** of **x**

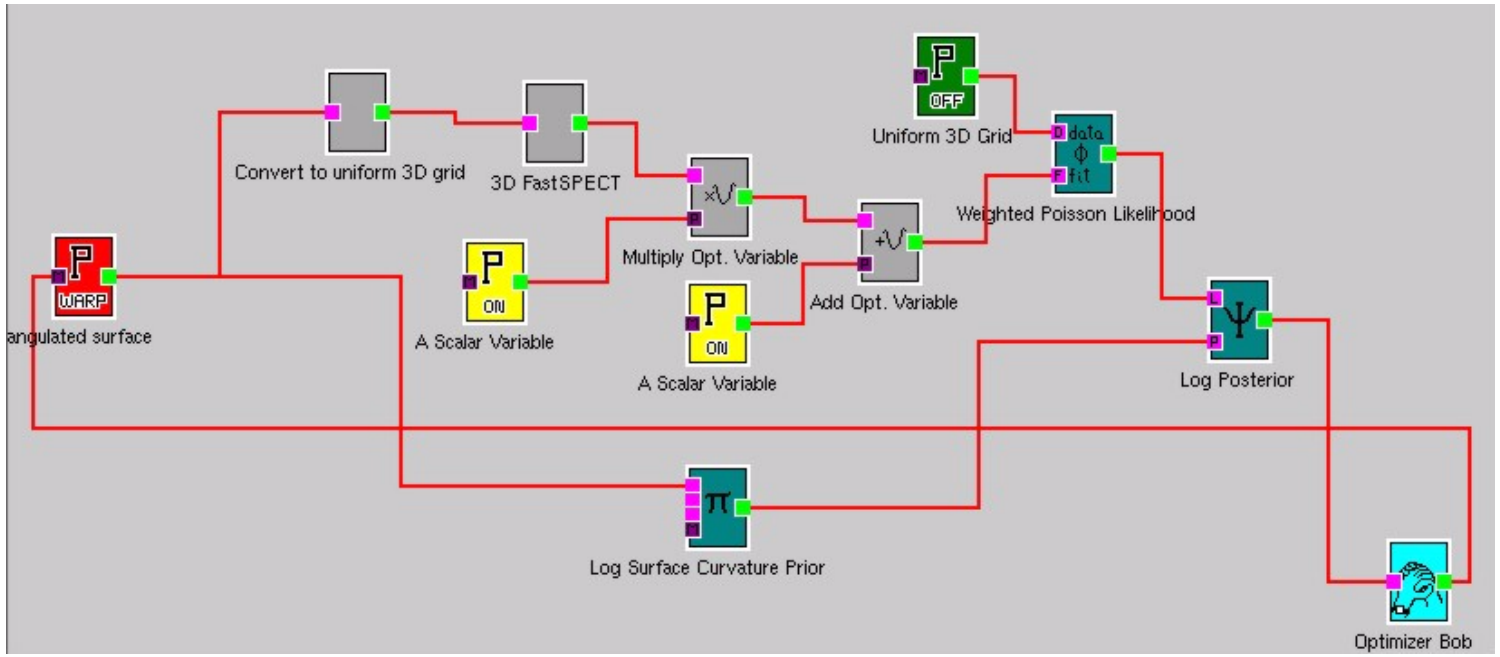
All derivatives computed in time comparable to forward calculation

Level of abstraction of implementation

- One can choose to differentiate forward code at various levels of abstraction - from coarse to fine
  - analytic-model based
    - e.g., differentiate partial differential equations and solve
    - not advised because forward codes only approximates model
  - algorithm based
    - differentiate each algorithm (e.g., Bayes Inference Engine)
  - code based
    - interpret programming code (FORTRAN, C, etc.)
    - automatic differentiation utilities
  - instruction based
    - reverse sequence of CPU instructions

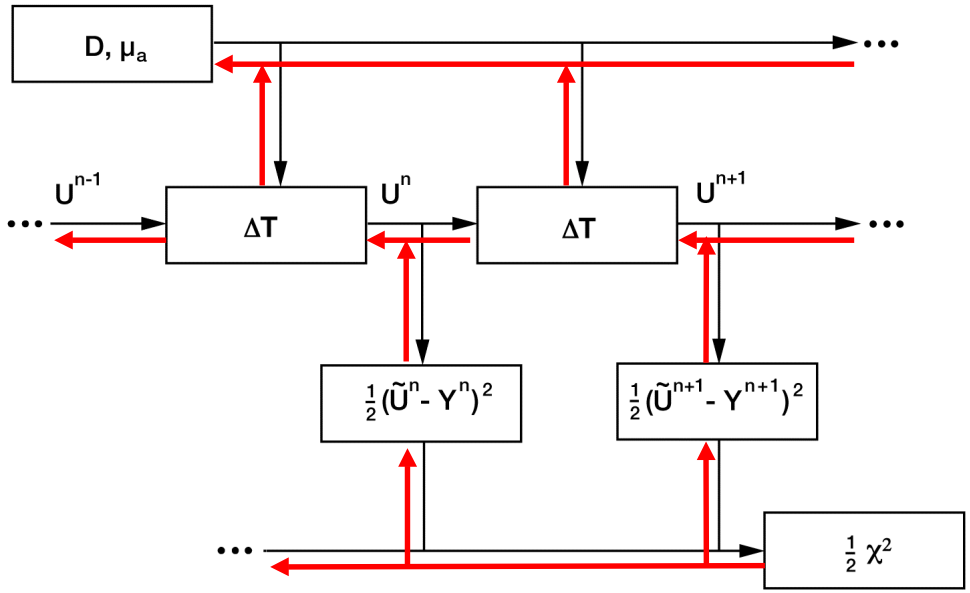
Example of algorithm-based approach

- Bayes Inference Engine (BIE) created at LANL
  - modeling tool for interpreting radiographs
  - BIE programmed by creating data-flow diagram liking transforms, as shown here for 3D reconstruction problem
- **Adjoint differentiation crucial to BIE success**



Adjoint differentiation in diffusion calculation

- Adjoint differentiation calculation **precisely reverses** direction of forward calculation
- Each forward data structure has an associated derivative
  - where $\mathbf{U}_n$ propagates forward, $\dfrac{\partial \varphi}{\partial \mathbf{U}_n}$ goes backward $\left(\varphi = \frac{1}{2}\chi^2\right)$



Adjoint differentiation of forward calculation

- Differentiate objective function, minus-log-likelihood:

$$\varphi(\alpha) = -\ln p(\mathbf{Y} \mid \alpha) = \tfrac{1}{2} \sum_m \frac{(Y_m - U_{s,n})^2}{\sigma_m^2} = \tfrac{1}{2} \chi^2$$

  - where $U_{s,n}$ is at the position s and time n corresponding to the mth measurement

- Derivative wrt each $U_{s,n}$ that contributes to the mth measurement is

$$\frac{\partial \varphi}{\partial U_{s,n}} = -\frac{Y_m - U_{s,n}}{\sigma_m^2}$$

Adjoint differentiation of forward calculation

- Sensitivity of $\varphi = \frac{1}{2}\chi^2$ wrt parameters $\alpha_i = (D \text{ or } \mu_a)_i$

$$\frac{d\varphi}{d\alpha_k} = \sum_{i,n} \frac{d\varphi}{dU_{i,n}} \frac{\partial U_{i,n}}{\partial \alpha_k}$$

- Get second factor from update formula

$$\mathbf{A}\mathbf{U}_n = \mathbf{U}_{n-1} + a\,\mathbf{S}_n$$

- For explicit α_k sensitivity, differentiate wrt α_k, taking $\mathbf{U}_{n-1}$ as constant:

$$\frac{\partial \mathbf{A}}{\partial \alpha_k}\mathbf{U}_n + \mathbf{A}\frac{\partial \mathbf{U}_n}{\partial \alpha_k} = 0$$

which leads to

$$\frac{\partial \mathbf{U}_n}{\partial \alpha_k} = -\mathbf{A}^{-1}\frac{\partial \mathbf{A}}{\partial \alpha_k}\mathbf{U}_n$$

Adjoint differentiation of forward calculation

- Dependence of $\mathbf{U}_{n+1}$ on $\mathbf{U}_n$ comes from update formula

$$\mathbf{A}\mathbf{U}_{n+1} = \mathbf{U}_n + a\,\mathbf{S}_n$$

- Differentiate wrt $\mathbf{U}_{n+1}$: $\dfrac{\partial \mathbf{U}_{n+1}}{\partial \mathbf{U}_n} = \mathbf{A}^{-1}$

- Total derivative of φ wrt $\mathbf{U}_n$ yields propagation rule

$$\frac{d\varphi}{d\mathbf{U}_n} = \left[\frac{d\mathbf{U}_{n+1}}{d\mathbf{U}_n}\right]^{\mathrm{T}} \frac{d\varphi}{d\mathbf{U}_{n+1}} + \frac{\partial\varphi}{\partial\mathbf{U}_n} = \left[\mathbf{A}^{-1}\right]^{\mathrm{T}} \frac{d\varphi}{d\mathbf{U}_{n+1}} + \frac{\partial\varphi}{\partial\mathbf{U}_n}$$

  - second term is derivative of φ wrt $\mathbf{U}_n$ when all other parameters are held constant
  - first term for $\mathbf{U}_n$ variation arising from other parameters

Comments about diffusion problem

- Algorithm used to solve forward problem was chosen without regard to inversion process
  - adjoint differentiation typically places minimal requirement on simulation method
- Simplifying aspects of diffusion problem:
  - update operation depends only on parameters $D(x,y)$ and $\mu_{abs}(x,y)$ (time independent)

Bayesian approach to inversion

- Inverse problems are often ill posed, meaning there is no unique solution
- Bayesian formalism overcomes ill posedness by introducing prior information through Bayes law:

$$\ln p(\alpha \mid \mathbf{Y}) = \ln p(\mathbf{Y} \mid \alpha) + \ln p(\alpha) + C$$

  - where $p(\alpha|\mathbf{Y})$ = posterior probability of the parameters α,
    $p(\mathbf{Y}|\alpha)$ = likelihood of the data,
    $p(\alpha)$ = prior probability of the parameters α
- Bayesian posterior $p(\alpha|\mathbf{Y})$ describes uncertainty in inferred parameters

Prior based on Markov Random Field model

- MRF can control local behavior of an intensity field
- Minus-log-prior given by (considering only D)

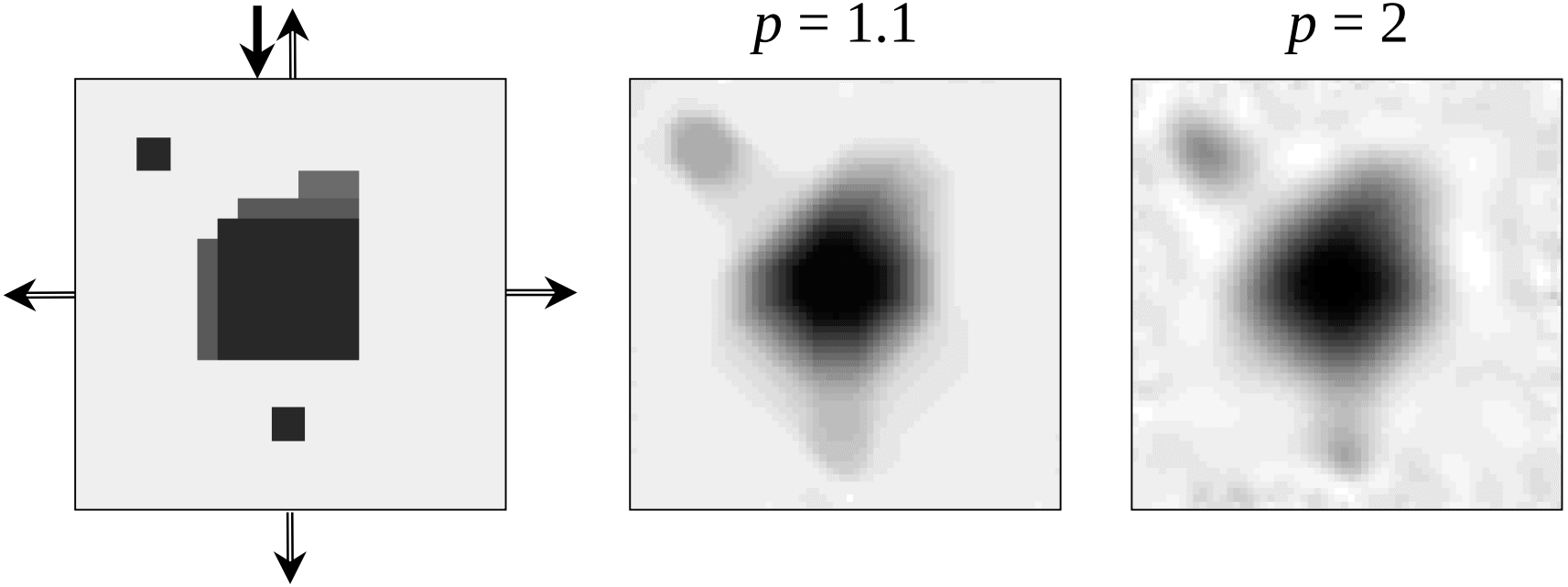
$$-\ln p(\mathbf{D}) = \beta \sum_i | D_i - \overline{D}_i |^p$$

  - where D_i = diffusion coefficient at ith pixel,
    $\overline{D}_i$ = D averaged over a neighborhood of ith pixel
  - this is added to minus-log likelihood ($\chi^2/2$)
- The exponent p controls shape of penalty function
  - $p = 2$ (standard) excessively penalizes large fluctuations
  - $p \cong 1$ results in better reconstructions
- Parameter β conveniently determined for MRF model

Examples of OT reconstructions

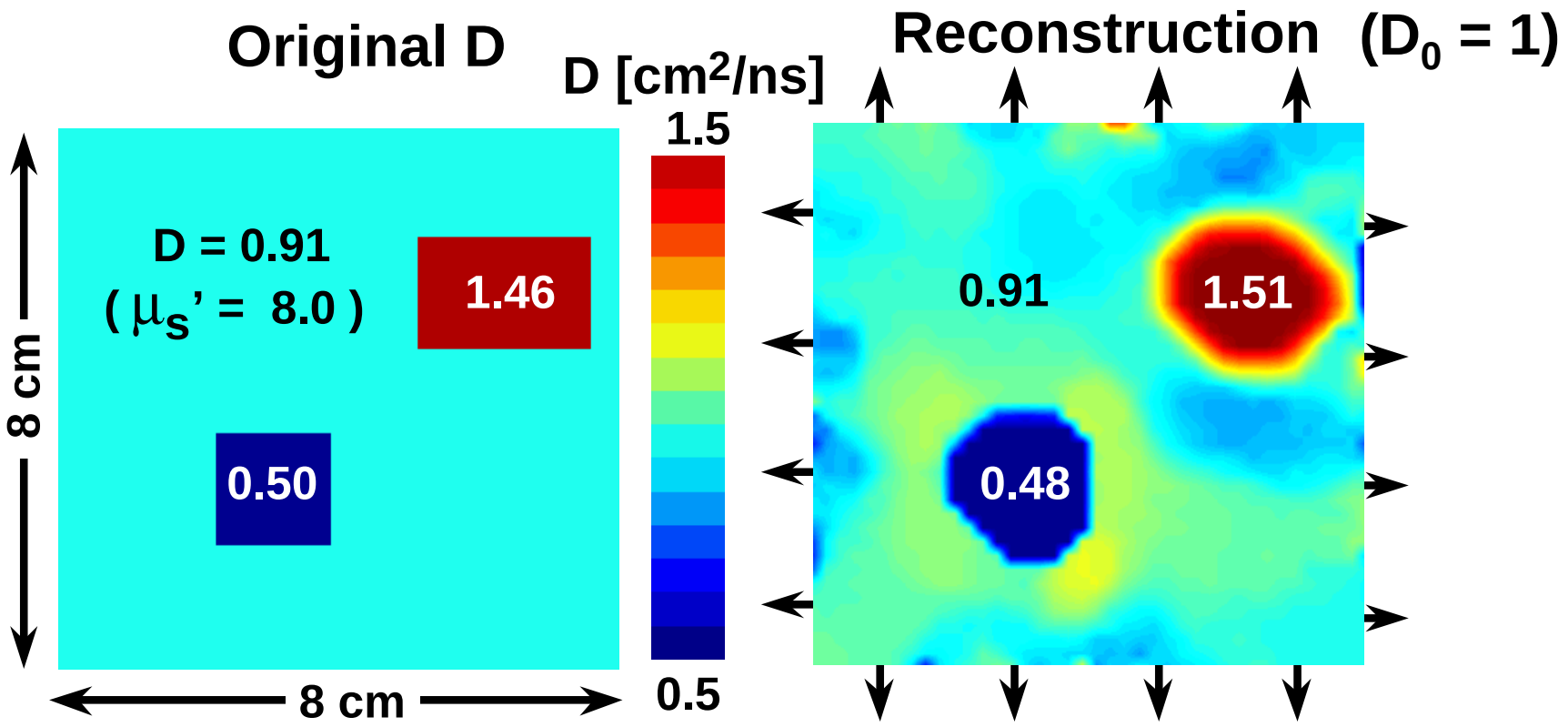
- Initial project - reconstruct $D(x,y)$ for simple phantom
  - Saquib, Hanson, Cunningham (LANL)
- Extension to simultaneously obtain $D(x,y)$ and $\mu_a(x,y)$; simulations relevant to human tissue
  - Hielscher, Klose, Catarious, Hanson (LANL)
- 3D reconstruction; applications to hypothetical diagnostic cases
  - brain, ventricular bleeding, and arthritis in finger joints
  - Hielscher, Klose (SUNY - Brooklyn), Hanson (LANL), Beuthan (FU Berlin)

Reconstruction of simple phantom



- Measurements
  - section is $(6.4\text{cm})^2$, $0.7 < D < 1.4$ $\text{cm}^2\text{ns}^{-1}$ ($\mu_{abs} = 0.1$ cm^{-1})
  - 4 input pulse locations (middle of each side)
  - 4 detector locations; intensity measured every 50 ps for 1 ns
- Reconstructions on 64 x 64 grid from noisy data (rmsn = 3%)
- Conjugate-gradient optimization algorithm

Simultaneously determine D and μ_a

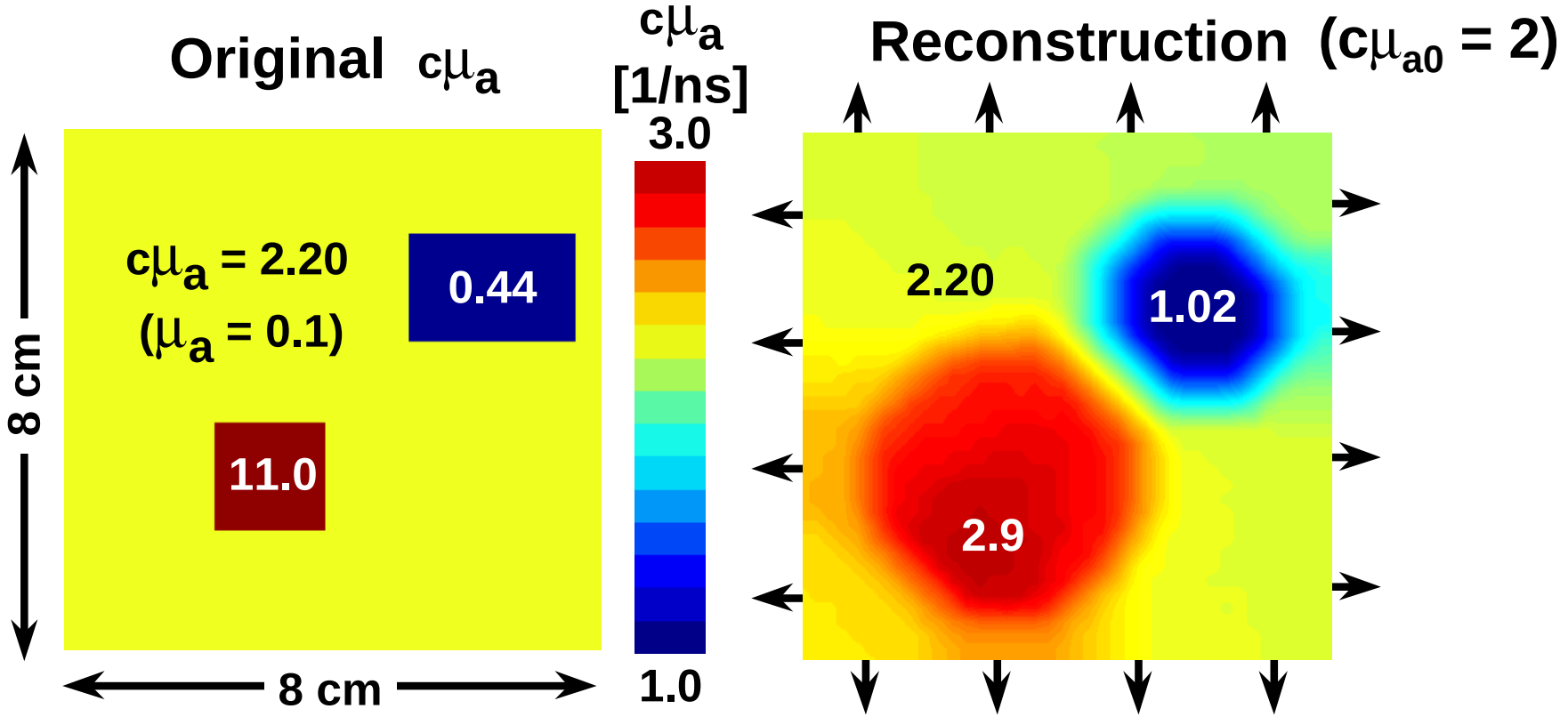


40x40 = 1600 pixels, 2 parameters;
16 sources and 15 detectors;
50 time steps

27 iterations ~ 8 min

Time for gradient calcs. for 27 iterations, relative to time for a single forward calc., = 16x27 = 432 by adj. diff.
1600x2x16x27 = 1,382,400 by finite diff.

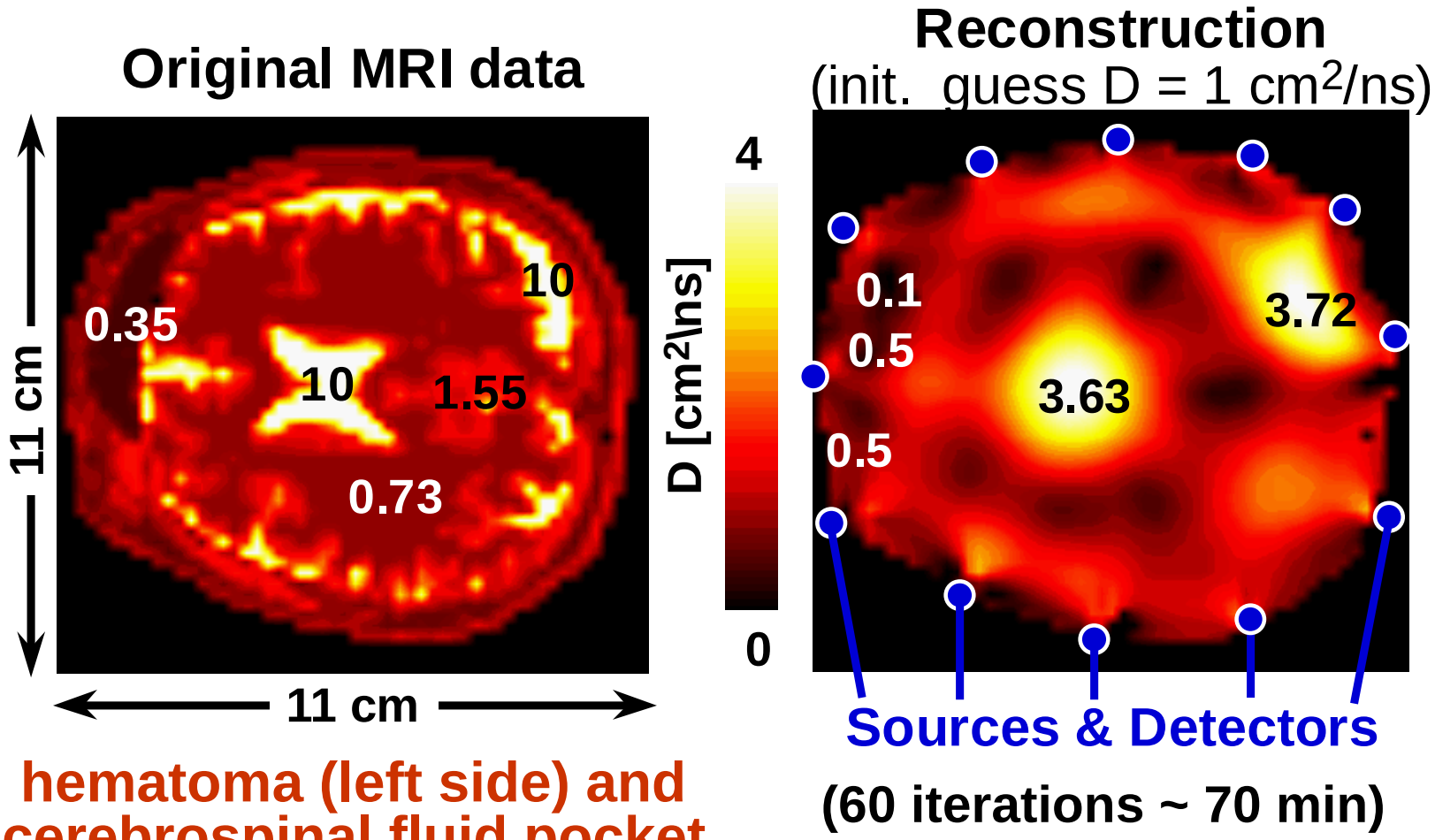
Simultaneously determine D and μ_a



40x40 = 1600 pixels, 2 parameters
16 source and 15 detector positions
50 time steps

27 iterations ~ 8 min

Reconstruction of Infant's Brain I

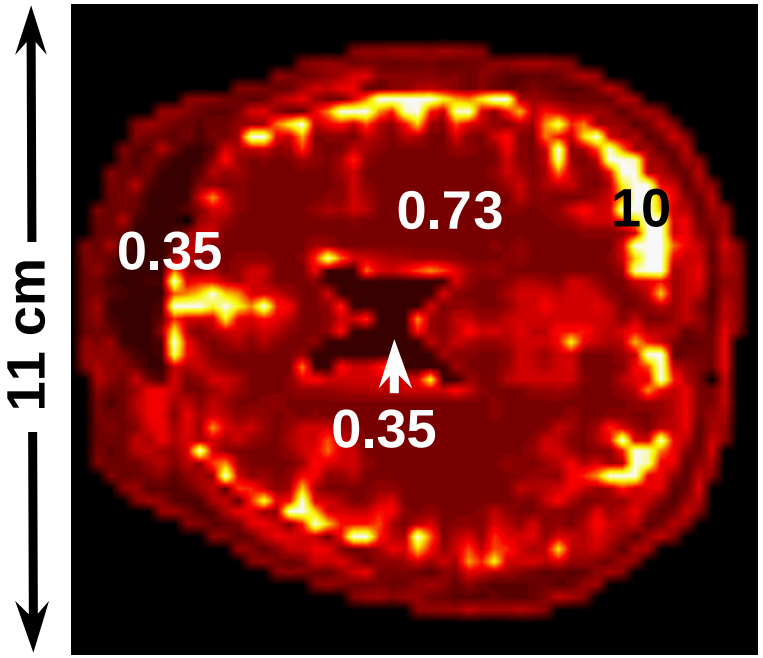


hematoma (left side) and cerebrospinal fluid pocket (upper right)

(60 iterations ~ 70 min)

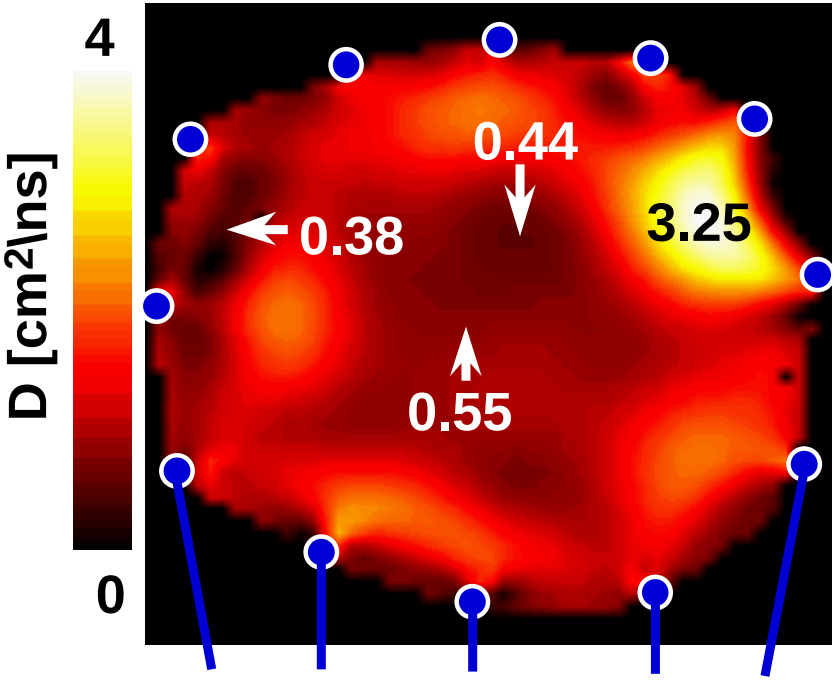
Reconstruction of Infant's Brain II

Original MRI data



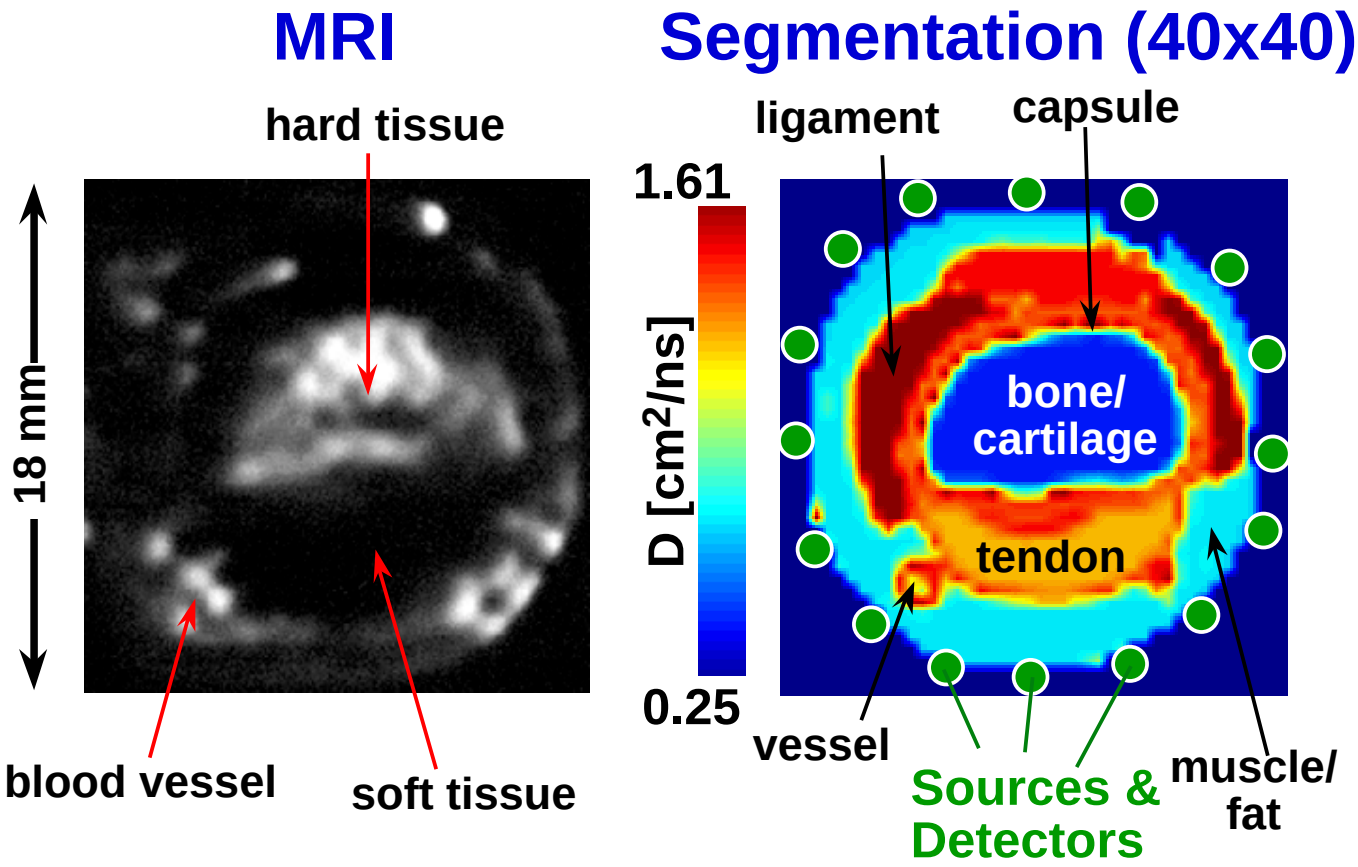
blood-filled ventricle (occurs in 15-30% of all preterm infants)

Reconstruction
(init. guess D = 1 cm^2/ns)



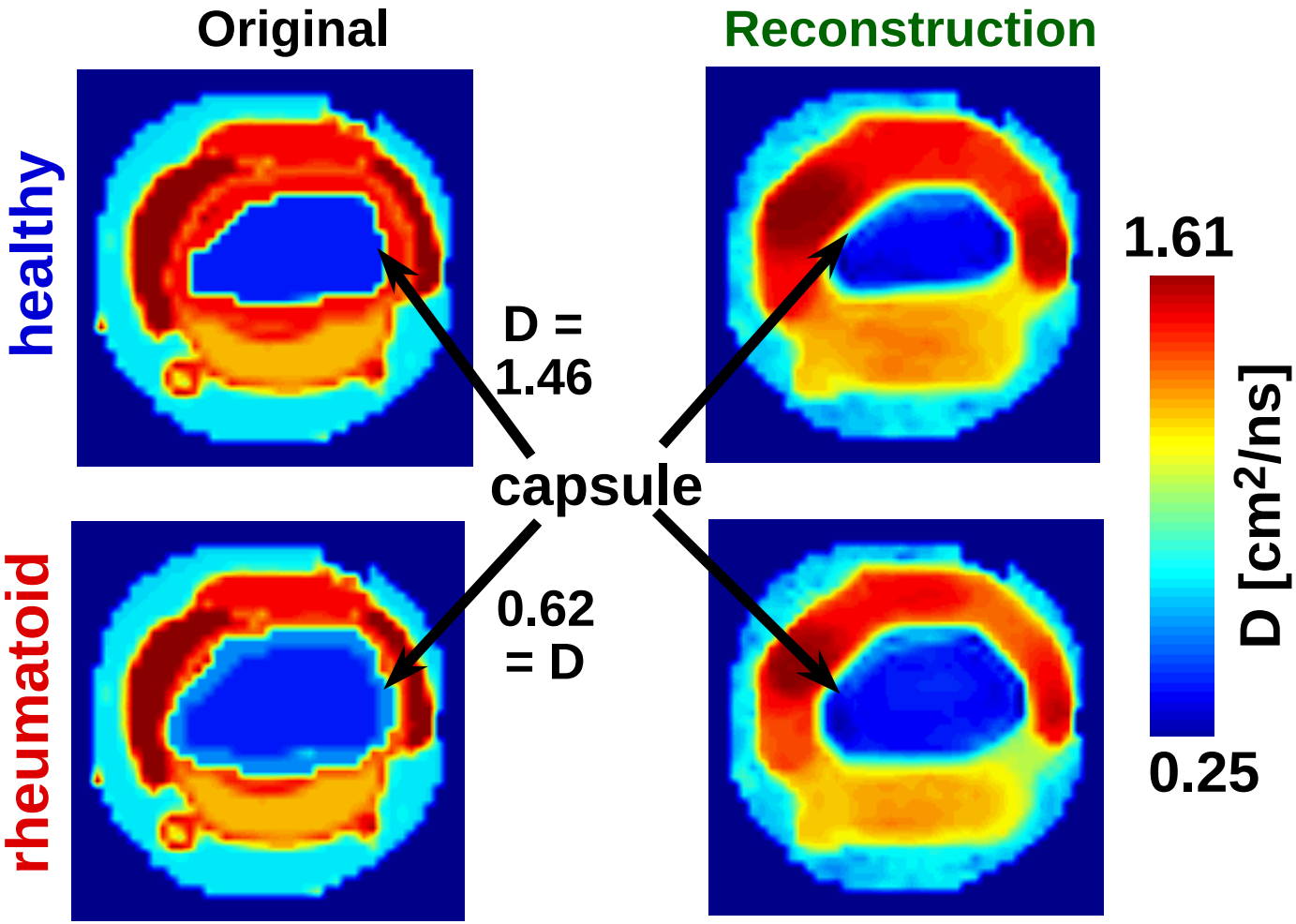
(60 iterations ~ 70 min)

Create Optical Image of Finger Joint

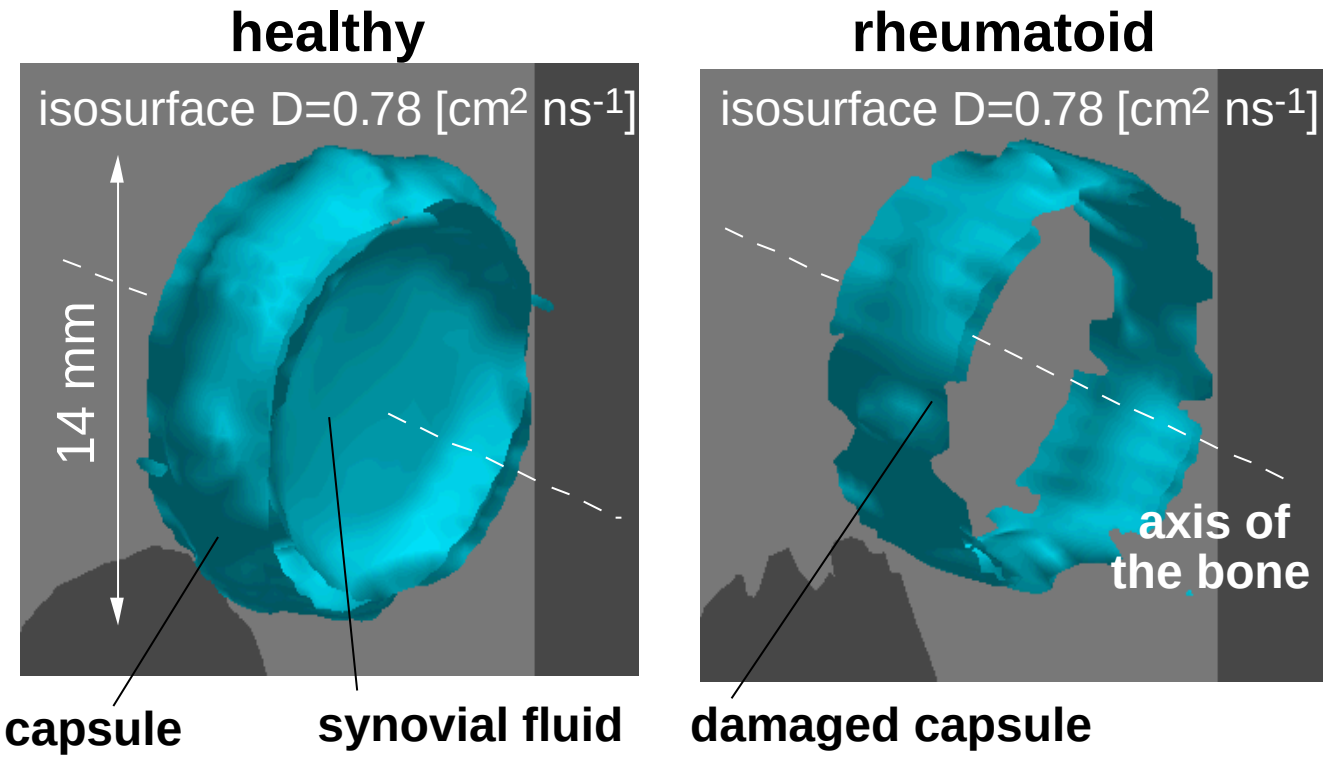


Simulated data obtained from optical image for source and detector positions shown

Reconstruction of Capsule



3D Reconstruction of Capsule



3D volume: 9 x 30 x 30 = 8100 voxels
8 sources x 8 detectors x 4 layers

Summary

- Propagation of light in tissue modeled as diffusion process
- Solve forward problem using finite-difference, implicit method
- Diffusion coefficients determined by matching simulated to actual measurements
- Adjoint differentiation essential to solution by providing gradients with respect to diffusion coefficients at cost of only one extra forward calculation
- Adjoint differentiation is generally useful when objective function is differentiable

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- "Inversion based on computational simulations," K. M. Hanson, et al., in *Maximum Entropy and Bayesian Methods*, pp. 121-135 (Kluwer, 1998)
- "Model-based image reconstruction from time-resolved diffusion data," S. S. Saquib, et al., *Proc. SPIE* **3034**, pp. 369-380 (1997)
- "Gradient-based iterative image reconstruction scheme for time-resolved optical tomography," A. H. Hielscher, et al., *IEEE Trans. Med. Imag.* **18**, pp. 262-271 (1999)
- "Two- and three-dimensional optical tomography of finger joints for diagnostics of rheumatoid arthritis," A. D. Klose, et al., *Proc. SPIE* **3566** (1998)

Find these under author's home page http://www.lanl.gov/home/kmh/

References for adjoint differentiation

- "Adjoint differentiation of hydrodynamic codes," M. L. Rightley et al., in CNLS Research Highlights, April, 1998 (http://public.lanl.gov/kmh/publications/CNLS97.pdf)
- “Recipes for adjoint code construction,” R. Giering et al., *ACM Trans. Math. Soft.* **24**, pp. 437-474 (1998). See also TAMC web pages below.

- Web sites for automatic differentiation packages:
  ADIFOR: http://www-unix.mcs.anl.gov/autodiff/ADIFOR/
  TAMC: http://klima47.dkrz.de/tamc/
  ODYSSEE: http//www.inria.fr/RRRT/RT-0224.html

Part 2 - More about adjoint differnentiation

- Other applications and uses of adjoint differentiation
- More about level of abstraction of implementation
- Automatic differentiation packages
- Use of check pointing to reduce resources needed to store forward solutions
- Interesting directions for future research

Further applications of adjoint differentiation

- Some significant applications under development
  - inversion of transport equation (A. Klose, FU Berlin)
  - oceanographics (Ralf Giering, JPL)
  - atmospherics (R. Errico, UCAR; R. Fovell, UCLA)
    - useful for simulations of up to several days
  - hydrodynamics (Rudy Henninger, LANL)

Potential uses of adjoint differentiation

- Reconstruction: imaging through refractive media
  - seismology, medical and NDE ultrasound, ...
- Matching large-scale simulations to data:
  - atmosphere and ocean models, fluid dynamics, hydrodynamic
- Optimization in large engineering design problems:
  - optical lens systems, geometry of integrated circuits, aerodynamic shape, engines
- Uncertainty analysis
  - sensitivity of uncertainty variance to each contributing cause
- Markov Chain Monte Carlo
  - generation of random samples from a prob. dens. function

Markov Chain Monte Carlo

- Generate random samples from a prob. dens. function
  - random walk around probability density function
- Simplest approach is based on evaluation of pdf (Metropolis)
  - efficiency drops for many variables ($\varepsilon \sim 0.3/n$)
- Gradient of pdf can improve efficiency
  - Langevin-Hastings algorithm
  - Hamiltonian hybrid method ($\varepsilon \sim$ independent of n)
- Gradient may be efficiently evaluated using adjoint differentiation

Further details about adjoint calculation

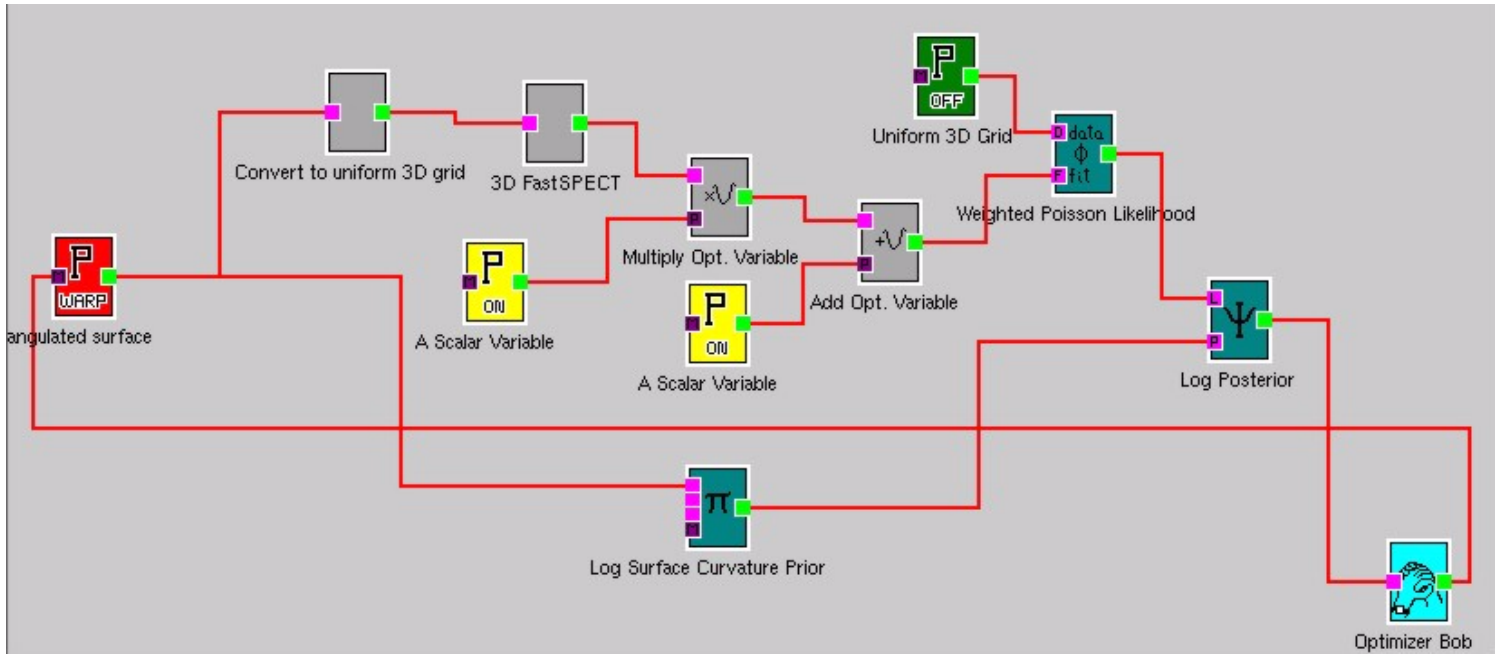
- Can be implemented a various levels of abstraction
- Automatic differentiation packages can be helpful
  - given forward code, provides an auxiliary code to calculate derivatives
  - potentially useful, but may require revising forward code
- Need to save variables from forward calculation implies huge storage requirements
  - check point the forward calculation; save intermediate results only occasionally

Level of abstraction of implementation

- One can choose to differentiate forward code at various levels of abstraction - from coarse to fine
  - analytic-model based
    - e.g., differentiate partial differential equations and solve
    - not advised because forward code only approximates model
  - algorithm based
    - differentiate each algorithm (e.g., Bayes Inference Engine)
  - code based
    - interpret programming code (FORTRAN, C, etc.)
    - automatic differentiation utilities
  - instruction based
    - reverse sequence of CPU instructions

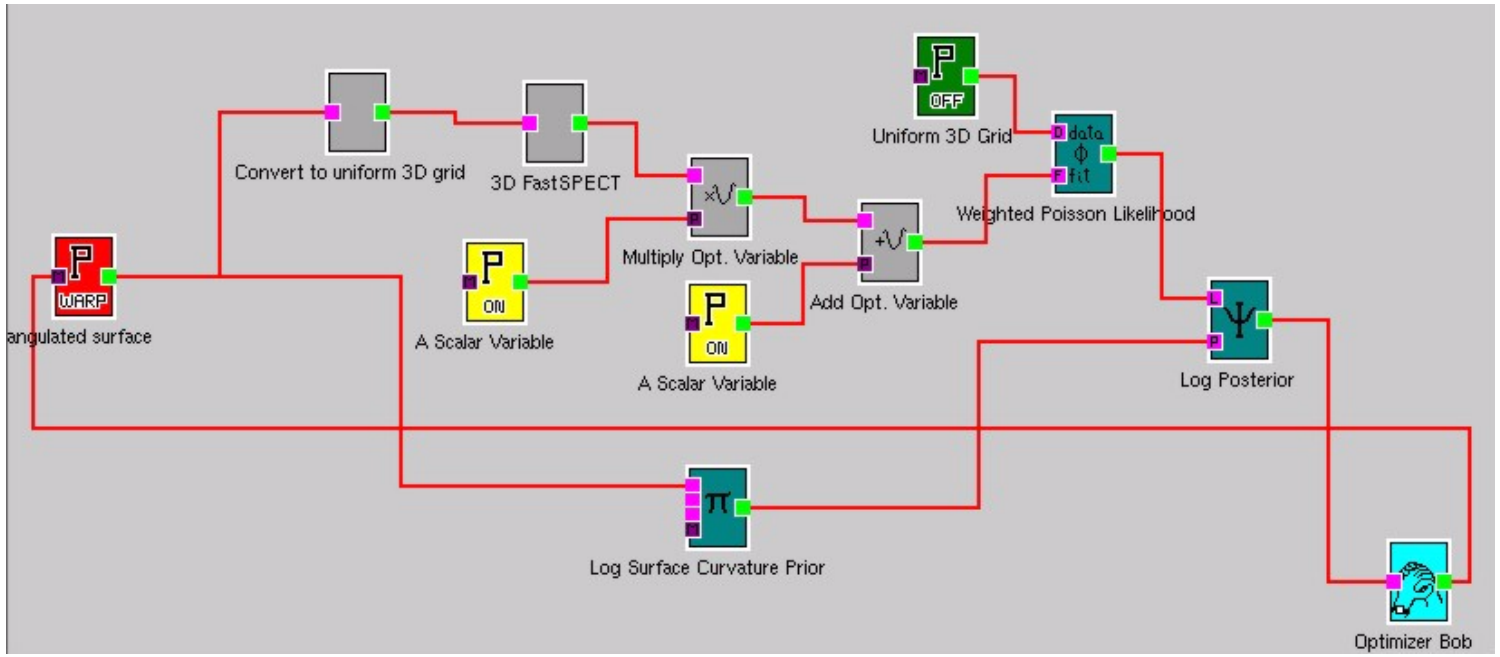
Example of algorithm-based approach

- Bayes Inference Engine (BIE) created at LANL
  - modeling tool for interpreting radiographs
  - BIE programmed by creating data-flow diagram, as shown here for 3D reconstruction problem
- **Adjoint differentiation crucial to BIE success**



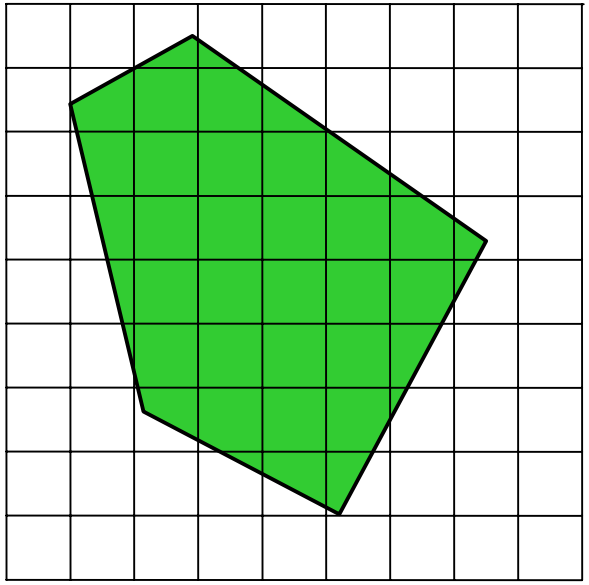
Bayes Inference Engine uses modules

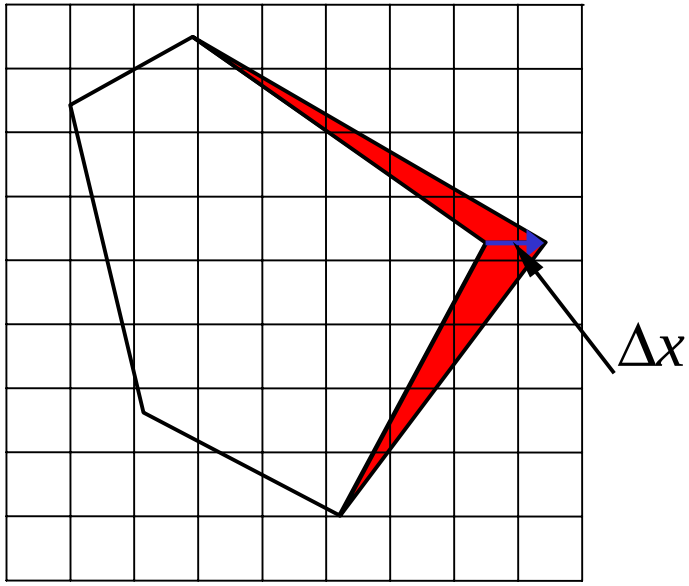
- Each module uses an algorithm to calculate:
  - its transform in forward direction
  - adjoint derivative in reverse direction (implemented as separate code)
- Optimizer (lower right)
  - gets objective function from log-posterior; provokes forward data flow
  - gets gradient from Parameter module; provokes reverse data flow



Example of algorithm-based approach

- Calculation of overlap of polyhedron with pixelated grid
  - green is area of overlap;
  - input is vertex positions, output is overlap with each pixel
- Derivative is limit of change in overlap caused by change in position of each vertex
  - example shown in red;
  - adjoint output is derivative of φ wrt vertex positions





Adjoint differentiation for linear transforms

– Linear transforms represented by matrix multiplications:

$$\mathbf{z} = \mathbf{B}\mathbf{A}\mathbf{x}$$
$$\varphi = |\mathbf{z} - \mathbf{c}|^2$$

where **z** and **x** are vectors containing the variables,
A and **B** are fixed matrices, and
c is a vector of constants (e.g., measurements)

– Derivative:

$$\frac{d\varphi}{d\mathbf{z}} = 2(\mathbf{z} - \mathbf{c})$$

$$\frac{d\varphi}{d\mathbf{x}} = \mathbf{A}^T\mathbf{B}^T\frac{d\varphi}{d\mathbf{z}} = \mathbf{A}^T\mathbf{B}^T 2(\mathbf{z} - \mathbf{c})$$

– For linear transforms, adjoint differentiation is the same as multiplication by the transpose of the matrix

Code-based forward derivative calculation

– Differentiate a few lines of FORTRAN code:

```
Y = EXP(A*X)
Z = B*Y*SIN(Y)
PHI = ALOG(Z*Z)
```

where `X`, `Y`, and `Z` are variables and `A` and `B` are constants

– The forward derivative code adds lines to forward code:

```
Y = A*X
DYDX = A*EXP(X)
Z = B*Y*SIN(Y)
DZDX = (B*SIN(Y) + B*Y*COS(Y))*DYDX
PHI = ALOG(Z*Z)
DPHIDX = (2.*Z)*(1./(Z*Z))*DZDX
```

– Similar to differentiation of analytic functions

Code-based adjoint calculation of derivatives

- Differentiate a few lines of FORTRAN code:

```
Y = EXP(A*X)
Z = B*Y*SIN(Y)
PHI = ALOG(Z*Z)
```

  where `X`, `Y`, and `Z` are variables and `A` and `B` are constants

- The reverse (adjoint) code looks like (note, `DPHIDX` is $\frac{\partial \varphi}{\partial x}$):

```
DPHIDZ = (2.*Z)*(1./(Z*Z))
DPHIDY = DPHIDZ*(B*SIN(Y) + B*Y*COS(Y))
DPHIDX = DPHIDY*A*EXP(X)
```

- forward code must be executed before adjoint code
- variables from forward calculation needed for adjoint calculation
- result for `DPHIDX` same as for forward calculation
- NB: this example is only meant to indicate how adjoint calculation is done; it is not particularly helpful in this situation

Code-based adjoint calculation of derivatives

- Differentiate a few lines of FORTRAN code:

```
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DPHIDZ = (2.*Z)*(1./(Z*Z))
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DPHIDX = DPHIDY*A*EXP(X)
```

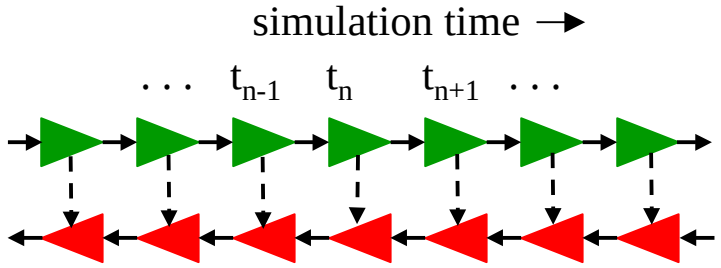
- forward code must be executed before adjoint code
- variables from forward calculation needed for adjoint calculation
- result for `DPHIDX` same as for forward calculation
- NB: this example is only meant to indicate how adjoint calculation is done; it is not particularly helpful in this situation

Automatic differentiation tools

- Several tools exist for automatically differentiating codes written in FORTRAN77
  - ADIFOR3 (Carle, Rice U; Bischof, Griewank, et al., ANL)
    - operates in both forward and reverse directions
    - works for large codes; follows ADICT principle
  - TAMC (R. Giering, JPL, prev. MIT & MPI-Meteorology)
    - operates in both forward and reverse directions
    - works for large codes; follows ADICT principle
  - GRESS (Hordewel, et al., ORNL)
    - operates in both forward and adjoint directions
    - can not compute gradients wrt many parameters for large calcs.
    - for adjoint, stores derivatives for each line of the forward code
  - ODYSSEE (INRIA, France)

Sequence of forward and adjoint calculations

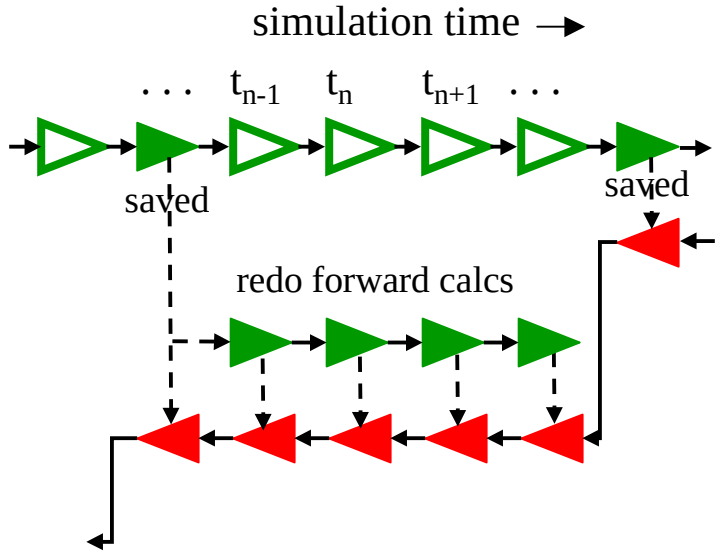
- Normal sequence for ADICT
  - first do full forward calculation (i.e., for all time steps)
  - then do full adjoint calculation in reverse direction, from final time back to beginning



- Adjoint calculation may need state of system from forward calculation
  - required link shown as vertical dashed lines
  - all necessary state variables must be saved from forward calculation to provide information to adjoint calculation

Check pointing forward results

- Adjoint calculation may need state of system from forward calculation
  - this requirement may exceed available memory
- Check pointing
  - first do full forward calc., **saving** state of system at selected times
  - then do adjoint calc. piecewise, repeating forward calc. to obtain states intermediate to those saved
  - trades off memory for compute time (for N time steps save ~ $\sqrt{N}$ storage for one extra forward calc.)



Potential extensions of adjoint differentiation

- Higher order derivatives
  - $\frac{\partial^2 \varphi}{\partial x_i \partial x_j}$ requires 2 forward and 2 adjoint calculations
  - large intermediate matrices => restrict to $\sum_j \frac{\partial^2 \varphi}{\partial x_i \partial x_j} x_j$
- Incorporate derivatives into data structures
  - with each variable vector **x**, associate $\delta \mathbf{x}$ and $\partial / \partial \mathbf{x}$
  - for each transformation $f(\mathbf{x})$, associate $\frac{\partial f}{\partial \mathbf{x}}$ with capabilities for forward and adjoint propagation
  - useful in symbolic languages, such as Maple (S. Gull)
  - facilitated in object-oriented setting (Bayes Inference Engine)
- Construct new programming paradigm based on these composite data structures in OO environment
  - view computer code as establishing links between transforms