SUNDIALS: SUite of Nonlinear and DIfferential / ALgebraic Equation Solvers

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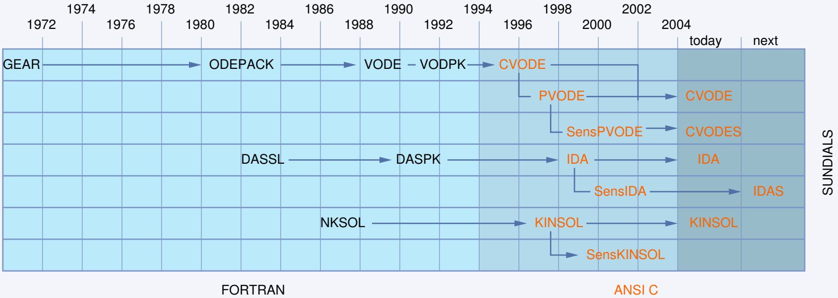
Outline

Outline

Historical background



Solution of large systems in parallel motivated writing (or rewriting) solvers in C

- **CVODE** C rewrite of **VODE**/**VODPK** [Cohen, Hindmarsh, 1994]
- **PVODE** parallel extension of **CVODE** [Byrne, Hindmarsh, 1998]
- **KINSOL** C rewrite of **NKSOL** [Taylor, Hindmarsh, 1998]
- **IDA** C rewrite of **DASPK** [Hindmarsh, Taylor, 1999]

New sensitivity capable solvers in SUNDIALS

- **CVODES** [Hindmarsh, S., 2002]
- **IDAS** [S., in development]

The SUNDIALS solvers

CVODE - ODE solver

- Variable-order, variable-step BDF (stiff) or implicit Adams (nonstiff)
- Nonlinear systems solved by Newton or functional iteration
- Linear systems solved by direct (dense or band) or iterative solvers

IDA - DAE solver

- Variable-order, variable-step BDF
- Nonlinear system solved by Newton iteration
- Linear systems solved by direct or iterative solvers

KINSOL - nonlinear solver

- Inexact Newton method
- Krylov solver: SPGMR (Scaled Preconditioned GMRES)

CVODES

- Sensitivity-capable (forward & adjoint) version of **CVODE**

IDAS

- Sensitivity-capable (forward & adjoint) version of **IDA**

Salient features of SUNDIALS solvers

- Philosophy: **Keep codes simple to use**
- Written in C
  - Fortran interfaces: **FCVODE** and **FKINSOL** (**FIDA** in development)
  - Matlab interfaces: **SUNDIALSTB** (**CVODES** and **KINSOL**)
- Written in a **data structure neutral** manner
  - No specific assumptions about data
  - Alternative data representations and operations can be provided
- Modular implementation
  - Vector modules
  - Linear solver modules
  - Preconditioner modules
- Require minimal problem information, but offer user control over most parameters

Outline

General form of an IVP

CASC

$$F(\dot{x}, x) = 0$$
$$x(t_0) = x_0$$

Definition

If $\partial F / \partial \dot{x}$ is invertible, we can formally solve for $\dot{x}$ to obtain an *ordinary differential equation* (ODE). Otherwise, we have a *differential algebraic equation* (DAE).

DAE as differential equations on manifolds (Rheinboldt, 1984)

$$\dot{x} = v(x) \, ; \quad x \in \mathcal{M}$$

Manifold: $\mathcal{M} = \{x \in R^n \mid g(x) = 0\}$

Tangent space: $T_x\mathcal{M} = \{v \in R^n \mid g_x(x)v = 0\}$

Vector field on $\mathcal{M}$: $v : \mathcal{M} \to R^n \, ; \quad \forall x \in \mathcal{M} \Rightarrow v(x) \in T_x\mathcal{M}$

DAE index

DAEs are best classified using various concepts of their *index*.

- the index of nilpotency (for linear constant coefficient DAE): measure of numerical difficulty in solving the DAE
- the differentiation index: "departure" from ODEs
- the perturbation index: measure of sensitivity of the solutions with respect to perturbations.
- ...

Definition (Gear & Petzold, 1983)

Equation $F(x, \dot{x})$ has *differentiation* index $\text{di} = m$ if m is the minimal number of analytical differentiations

$$F(\dot{x}, x) = 0, \ \frac{dF(\dot{x}, x)}{dt} = 0, \ \ldots, \ \frac{d^m F(\dot{x}, x)}{dt^m} = 0$$

such that, by algebraic manipulations, we can extract an explicit ODE $\dot{x} = \phi(x)$ (called "underlying ODE").

Hessenberg index-1

$$\dot{x} = f(x, z)$$
$$0 = g(x, z)$$

- g_z nonsingular
- Example: singular perturbation problems (e.g. chemical kinetics)

Robertson's example (1966)

$$A \xrightarrow[\text{(slow)}]{0.04} B$$
$$B + B \xrightarrow[\text{(very fast)}]{3\cdot 10^7} C + B$$
$$B + C \xrightarrow[\text{(fast)}]{10^4} A + B$$

$$\dot{y}_A = -0.04 y_A + 10^4 y_B y_C \; ; \qquad y_A(0) = 1$$
$$\dot{y}_B = 0.04 y_A - 10^4 y_B y_C - 3 \cdot 10^7 y_B^2 \; ; \qquad y_B(0) = 0$$
$$1 = y_A + y_B + y_C$$

Hessenberg index-2

$$\dot{x} = f(x, z)$$
$$0 = g(x)$$

- $g_x f_z$ nonsingular
- Example: modeling of incompressible fluid flow by Navier-Stokes

$$u_t + uu_x + vu_y + p_x - \nu(u_x x + u_y y) = 0$$
$$v_t + uv_x + vv_y + p_y - \nu(v_x x + v_y y) = 0$$
$$u_x + v_y = 0$$

with appropriate spatial discretization.

Stiff problems

Definition (Curtiss & Hirschfelder, 1952)

Stiff equations are equations where certain implicit methods, in particular BDF, perform better, usually tremendously better, than explicit ones.

- Stiffness can be defined in terms of *multiple time scales*: If the system has widely varying time scales, and the phenomena (or *solution modes*) that change on fast scales are **stable**, then the problem is stiff (Ascher & Petzold, 1998)
- Stiffness depends on
  - Jacobian eigenvalues
  - system dimension
  - accuracy requirements
  - length of simulation
  - ...
- In general, we say a problem is *stiff* on $[t_0, t_1]$, if

$$(t_1 - t_0) \min_j \Re(\lambda_j) \ll -1$$

Forward Euler vs. Backward Euler

- **Dahlquist test equation**

$$\dot{x} = \lambda x\,, \quad x_0 = 1$$

Exact solution: $y(t_n) = y_0 e^{\lambda t_n}$

- **Absolute stability requirement**

$$|y_n| \le |y_{n-1}|\,,\ n = 1, 2, \dots$$

Reason: If $\Re(\lambda) < 0$, then $|y(t_n)|$ decays exponentially. The problem is asymptotically stable, and we cannot tolerate growth in $|y(t_n)|$.

- **Region of absolute stability**

$$S = \{ z \in \mathbb{C};\ |R(z)| \le 1 \}$$

where $y_n = R(z) y_{n-1}\,,\ z = h\lambda$

- **Forward Euler**

$$y_n = y_{n-1} + h(\lambda y_{n-1}) \ \Rightarrow\ S = \{ z \in \mathbb{C};\ |z - (-1)| \le 1 \}$$

Step size restriction: if $\lambda < 0 \ \Rightarrow\ h \le \frac{2}{-\lambda}$

- **Backward Euler**

$$y_n = y_{n-1} + h(\lambda y_n) \ \Rightarrow\ S = \left\{ z \in \mathbb{C};\ |1 - z|^{-1} \le 1 \right\}$$

Step size restriction: if $\lambda < 0 \ \Rightarrow\ h > 0$

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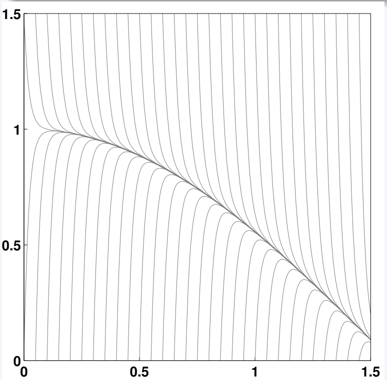
Curtiss & Hirschfelder example

$$\dot{x} = -50\,(x - \cos(t))$$



Solution curves

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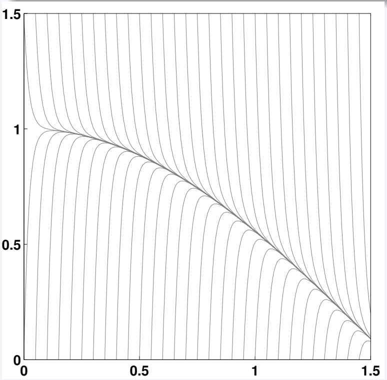

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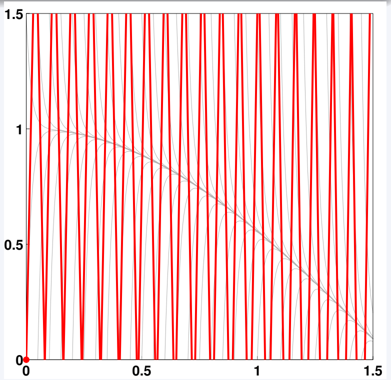

Forward Euler ($h = 2.01/50$)

Curtiss & Hirschfelder example

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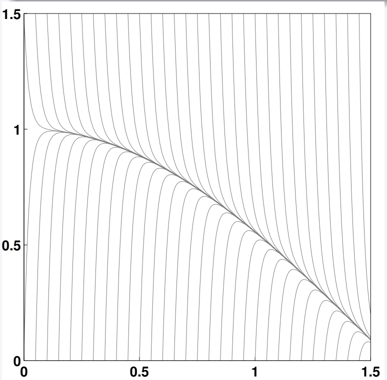

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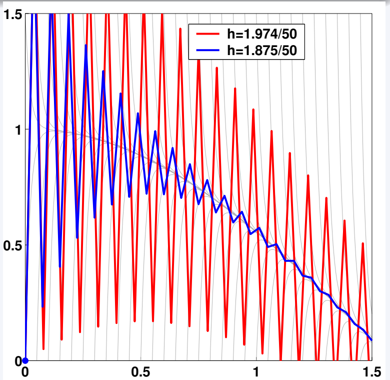

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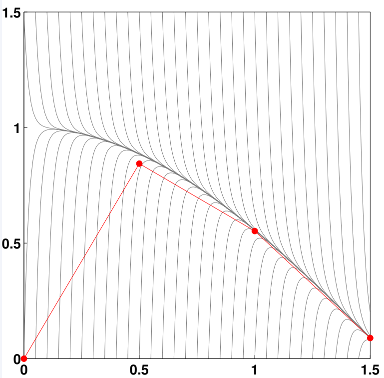
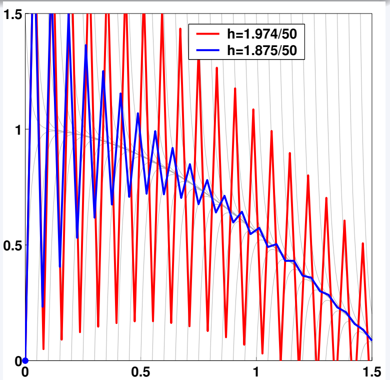


Backward Euler (3 steps)



Forward Euler

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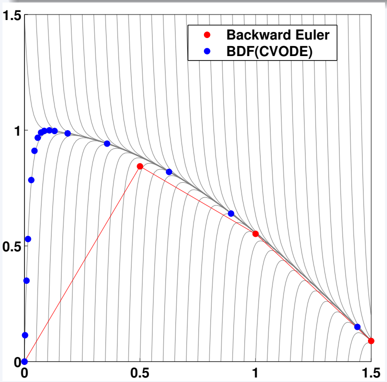
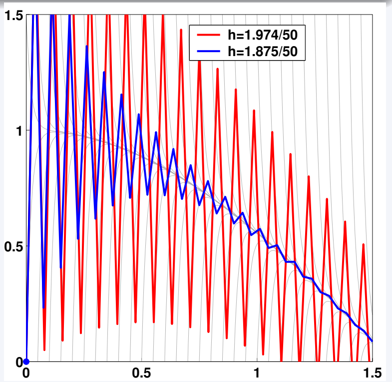


CVODE solution



Forward Euler

Linear multistep methods

General form

$$\sum_{i=0}^{K_1} \alpha_{n,i} x_{n-i} + h_n \sum_{i=0}^{K_2} \beta_{n,i} \dot{x}_{n-i} = 0$$

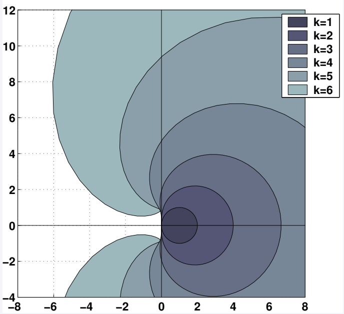
Two particular methods

- Adams-Moulton (nonstiff)
  $K_1 = 1, K_2 = k, k = 1, \ldots, 12$
- BDF (stiff)
  $K_1 = k, K_2 = 0, k = 1, \ldots, 5$

Nonlinear system (BDF)

- ODE: $\dot{x} = f(x)$
  $G(x_n) \equiv x_n - \beta_0 h_n f(x_n) - \sum_{i>0} \alpha_{n,i} x_{n-i} = 0$
- DAE: $F(\dot{x}, x) = 0$
  $G(x_n) \equiv F\left((\beta_0 h_n)^{-1} \sum_{i \geq 0} \alpha_{n,i} x_{n-i}, x_n \right) = 0$

BDF: $x_n - \beta_0 h_n \dot{x}_n = \sum_{i=1}^{k} \alpha_{n,i} x_{n-i}$



Absolute stability regions

LMM: variable-order, variable-step BDF

- **Fixed-leading coefficient form of BDF formulas**
- **Predictor-corrector implementation**
  - Predictor $x_{n(0)} = \sum_{i=1}^{k} \alpha_i^p x_{n-i} + \beta_0^p h_n \dot{x}_{n-1}$
  - Corrector $x_n = \sum_{i=1}^{k} \alpha_i x_{n-i} + \beta_0 h_n f(x_n)$
- **Use weighted residual mean square norms**

  $||x||_{\text{wrms}} := \sqrt{(x_i w_i)^2 / N} \quad w_i = \frac{1}{\text{rtol}|x_i| + \text{atol}_i}$
- **Error control mechanism**
  - Step size selection
    1. Estimate error: $E(h_n) = C \cdot (x_n - x_{n(0)})$
    2. Accept step if $||E(h_n)||_{\text{wrms}} < 1.0$
    3. Estimate error at next step $E(h'_n) \approx (h'_n / h_n)^k \, E(h_n)$
    4. Select h'_n such that $||E(h'_n)||_{\text{wrms}} < 1.0$
  - Method order selection
    1. Estimate errors for next higher and lower orders
    2. Select the order that gives the largest step size meeting the error condition

LMM: nonlinear system solution

CASC

- Use predicted value $x_n(0)$ as initial guess for the nonlinear iteration
- **Nonstiff systems: Functional iteration**

$$x_{n(m+1)} = \beta_0 h_n f\left(x_{n(m)}\right)$$

- **Stiff systems: Newton iteration**

$$M\left(x_{n(m+1)} - x_{n(m)}\right) = -G\left(x_{n(m)}\right)$$

  - ODE:
    $M \approx I - \partial f / \partial x$, $\gamma = \beta_0 h_n$
  - DAE:
    $M \approx \partial F / \partial y + \gamma \partial F / \partial \dot{x}$, $\gamma = 1/(\beta_0 h_n)$

LMM: linear system solution

- Direct dense
- Direct band
- Direct sparse
- Iterative linear solvers
  - Result in Inexact Newton nonlinear solver
  - Scaled preconditioned solvers: GMRES, Bi-CGStab, TFQMR
  - Only require matrix-vector products
  - Require preconditioner for the Newton matrix M
- Jacobian information (matrix or matrix-vector product) can be supplied by the user or estimated by difference quotients

Outline

1. SUNDIALS: overview
2. ODE and DAE integration
   - Initial value problems
   - Implicit integration methods
3. **Nonlinear systems**
   - Newton's method
   - Inexact Newton
   - Preconditioning
4. Sensitivity analysis
   - Definitions, applications, methods
   - Forward sensitivity analysis
   - Adjoint sensitivity analysis
5. SUNDIALS: usage, applications, availability
   - Usage
   - Applications
   - Availability

Basic method

CASC

$$F(x) = 0$$

x^0 : starting point

- Basis for most nonlinear solvers: Newton's method

$$J(x^k)\Delta x_k = -F(x^k) \quad \text{where } J(x) = F_x(x)$$
$$x^{k+1} = x^k + \Delta x_k$$

- Convergences if x^0 is *close enough* to x^* and $\exists J^{-1}(x^*)$
- Quadratic convergence: $\|x^{k+1} - x^*\| \leq C\|x^k - x^*\|$, for some $C > 0$

Modifications and enhancements

Two main problems with Newton's method:

- Need to calculate the Jacobian matrix
  - Matrix-free linear solvers
  - Multi-secant methods (Broyden)
    Use successive approximations B_k to the Jacobian matrix $J(x^k)$
- No guaranteed global convergence
  - Line search with backtracking
    Use only a fraction of the full Newton step: $x^{k+1} = x^k + \lambda \Delta x_k$
    Select λ to obtain
    - sufficient decrease in F relative to the step length
    - a minimum step length relative to the initial rate of decrease
    - full Newton step close to x^*.
  - Trust region methods

KINSOL provides *matrix-free linear solvers* and *line search with backtracking* capabilities.

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Inexact Newton

Solve linear systems *approximately*

$$F_x(x^k)\Delta x_k \approx -F(x^k)$$

$$\text{such that } \|F(x^k) + F_x(x^k)\Delta x_k\| \le \eta_k \|F(x^k)\|$$

$$x^{k+1} = x^k + \Delta x_k$$

Stopping tolerance η_k is selected to prevent "over-solves"

- Newton's method is based on a linear model
  - Bad approximation far from solution $\Rightarrow$ loose tolerances
  - Good approximation close to solution $\Rightarrow$ tight tolerances
- Eisenstat and Walker
  - Choice 1 $\quad \eta_k = \|F(x^k)\| - \|F(x^{k-1}) + F_x(x^{k-1})\Delta x_{k-1}\| / \|F(x^{k-1})\|$
  - Choice 2 $\quad \eta_k = 0.9\left(\|F(x^k)\| / \|F(x^{k-1})\|\right)^2$
- Constant value
  - Kelley $\quad \eta_k = 0.1$
  - ODE literature $\quad \eta_k = 0.05$

Preconditioned Krylov solver

Linear system within the Newton iteration: $Js = r$

- Krylov iterative methods find the solution in the subspace $K(J, r) = \{r, Jr, J^2r, \ldots\}$
- Their convergence rate depends on the spectral properties of J
- Preconditioning: replace the linear system with an equivalent one that has more favorable spectral properties
- Preconditioning on the right: $(JP^{-1})(Ps) = r$
- The preconditioner P must approximate the Jacobian matrix, yet be reasonably cheap to evaluate and efficient to solve
  - setup phase: evaluate and preprocess P (infrequent)
  - solve phase: solve systems $Px = b$ (frequent)
- Many preconditioner types
  - Jacobi preconditioner
  - Incomplete factorization preconditioners
  - Block preconditioners
  - Preconditioners based on the underlying problem

Outline

Definitions

Definition

Broadly speaking, *sensitivity analysis* (SA) is the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variation.

First-order SA problem (dynamical systems)

$$F(\dot{x}, x, p) = 0$$
$$y(p) = \mathcal{O}(x, p)$$

where $x \in R^n$ and $y \in R$ ($\mathcal{O} : R^n \times R^{N_p} \to R$).
Considering the Taylor expansion of y around the nominal value p

$$y(p + \delta p) = y(p) + \nabla_p y(p) \cdot \delta p + O(\delta p^2)$$

we define the first-order SA problem as the problem of computing the gradient $\nabla_p y$.

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Applications of SA

- **Model evaluation**
  Finding most and least influential parameters
- **Model reduction**
  Reducing model complexity, while preserving its input-output behavior
- **Data assimilation**
  Merging observed information into a model in order to improve its accuracy
- **Uncertainty quantification**
  Characterizing (quantitatively) and reducing uncertainty in model predictions
- **Dynamically-constrained optimization**
  Improving model response (better performance, better agreement with observations, etc.)

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Methods

Parameter-dependent ODE system

Model: $F(\dot{x}, x, p) = 0$

Output functional: $y(p) = \mathcal{O}(x, p)$

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DSA - discrete sensitivity analysis

$$\frac{dy}{dp_i}(p) \approx \frac{y(p + e_i \delta p_i) - y(p)}{\delta p_i}$$

or

$$\frac{dy}{dp_i}(p) \approx \frac{y(p + e_i \delta p_i) - y(p - e_i \delta p_i)}{2\delta p_i}$$

e_i is the i-th column of the identity matrix and δp is a vector of perturbations.

Methods

Parameter-dependent ODE system

Model: $F(\dot{x}, x, p) = 0$

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FSA

$$F_{\dot{x}} \dot{s}_i + F_x s_i + F_{p_i} = 0$$

and

$$\nabla_p y(p) = [\cdots, \mathcal{O}_x s_i + \mathcal{O}_{p_i}, \cdots]$$

Cost: $(1 + N_p) \times \mathrm{cost}(\mathcal{M})$

ASA

$$(\lambda^* F_{\dot{x}})' - \lambda^* F_x = -\mathcal{O}_x^* 1$$

and

$$\nabla_p y(p) = \langle F_p, \lambda \rangle + \mathcal{O}_p$$

Cost: $(1 + N_y) \times \mathrm{cost}(\mathcal{M})$

Methods

CASC

Parameter-dependent ODE system

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FSA for ODE and DAE systems

- Parameter dependent system: $F(\dot{x}, x, p) = 0\,, \quad x(t_0) = x_0(p)$
- Output functional: $g(x, p)$
- Sensitivity systems: $(i = 1, 2, \ldots, N_p)$

$$F_{\dot{x}} \dot{s}_i + F_x s_i + F_{p_i} = 0\,, \quad s_i(t_0) = x_{0p_i}$$

- Gradient of output functional:

$$\nabla_p g = g_x s + g_p$$

where $s = [s_1, s_2, \ldots, s_{N_p}]$ is the *sensitivity matrix*

Good: Sensitivity system does *not* depend on $\mathcal{O}$
Bad: Sensitivity system depends on p

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FSA: generation of the sensitivity system

$$\dot{x} = f(x,p) \quad \Rightarrow \quad \dot{s}_i = f_x s_i + f_{p_i}$$

- Analytical
- AD (ADIFOR, ADIC, ADOLC, ...)
- Directional derivative approximations

$$\begin{cases} f_x s_i \approx \frac{f(t,x+\sigma_x s_i,p) - f(t,x-\sigma_x s_i,p)}{2\sigma_x} \\ f_{p_i} \approx \frac{f(t,x,p+\sigma_i e_i p) - f(t,x,p-\sigma_i e_i)}{2\sigma_i} \end{cases} \qquad \begin{cases} \sigma_i = |\bar{p}_i| \sqrt{\max(rtol,\epsilon)} \\ \sigma_x = \frac{1}{\max(1/\sigma_i, \|s_i\|_{WRMS}/|\bar{p}_i|)} \end{cases}$$

or

$$f_x s_i + f_{p_i} \approx \frac{f(t, x+\sigma s_i, p+\sigma e_i p) - f(t, x-\sigma s_i, p-\sigma e_i)}{2\sigma}$$

where $\sigma = \min(\sigma_i, \sigma_x)$

FSA: implementation issues

Must take advantage of the shared structure with original system

Solutions (for implicit ODE/DAE integrators)

- **Staggered Direct** (Caracotsios & Stewart, 1985):
  iterate to convergence the nonlinear state system and then solve the linear sensitivity systems
  requires formation and storage of J; errors in J → errors in s
- **Simultaneous Corrector** (Maly & Petzold, 1997):
  solve simultaneously a nonlinear system for both states and sensitivity variables
  requires formation of sensitivity r.h.s. at every iteration
- **Staggered Corrector** (Feehery, Tolsma, Barton, 1997):
  iterate to convergence the nonlinear state system and then use a Newton method to solve for the sensitivity variables
  with iterative linear solvers → effectively Staggered Direct

CVODES and **IDAS** implement the *simultaneous corrector* and two flavors of the *staggered corrector* approaches.

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CVODES and **IDAS** implement the *simultaneous corrector* and two flavors of the *staggered corrector* approaches.

Speedup results for FSA

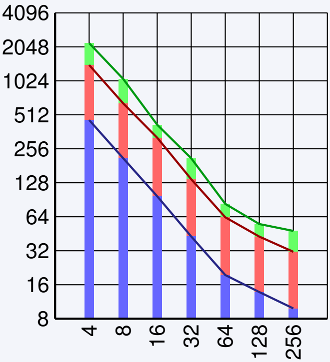
CASC

Problem 2-species 2D diurnal kinetics advection-diffusion PDE system.

Dimension $N = 2 \cdot (p_x n_x) \cdot (p_z n_z) = 2 \cdot 1600 \cdot 400 = 1280000$

Platform Parallel performance tests were performed on ASCI Frost, a 68-node, 16-way SMP system with POWER3 375 MHz processors and 16 GB of memory per node.

P ($p_x p_z$)	CPU time (s): States only	CPU time (s): Staggered partial	CPU time (s): Staggered full
4	460.31	1414.53	2208.14
8	211.20	646.59	1064.94
16	97.16	320.78	417.95
32	42.78	137.51	210.84
64	19.50	63.34	83.24
128	13.78	42.71	55.17
256	9.87	31.33	47.95



ASA - ODE derivation

- Parameter dependent system: $F(\dot{x}, x, p) = 0\,, \quad x(t_0) = x_0(p)$
- Output functional: $G(p) = \int_{t_0}^{t_f} g(x,p)\, dt$

  $\nabla_p G = \int_{t_0}^{t_f} (g_x s + g_p)\, dt + \int_{t_0}^{t_f} \lambda^* \left(F_{\dot{x}} \dot{s} + F_x s + F_p\right)\, dt$

  $= \int_{t_0}^{t_f} (g_x + (\lambda^* F_{\dot{x}})' - \lambda^* F_x)\, s\, dt + \int_{t_0}^{t_f} (g_p - \lambda^* F_p)\, dt - (\lambda^* F_{\dot{x}} s)|_{t_0}^{t_f}$
- Adjoint system:

$$(\lambda^* F_{\dot{x}})' - \lambda^* F_x + g_x = 0\,, \quad (\lambda^* F_{\dot{x}})|_{t_f} = ?$$

- Gradient of output functional:

$$\nabla_p G = \int_{t_0}^{t_f} (g_p - \lambda^* F_p)\, dt - (\lambda^* F_{\dot{x}} s)_{t=t_f} + (\lambda^* F_{\dot{x}})_{t=t_0} x_{0p}$$

Good: Sensitivity system does *not* depend on p
Bad: Sensitivity system depends on $\mathcal{O}$

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Output functional: $G(p) = \int_{t_0}^{t_f} g(x, p)\, dt$

Gradient: $\nabla_p G = \int_{t_0}^{t_f} (g_p - \lambda^* F_p)\, dt - (\lambda^* F_{\dot{x}} x_p)\big|_{t_0}^{t_f}$

Adjoint system: $(\lambda^* F_{\dot{x}})' - \lambda^* F_x = -g_x\,, \quad \lambda^* F_{\dot{x}}\big|_{t_f} = ?$

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index-0 and index-1 DAE

$$F(\dot{x}, x) = 0 \Rightarrow (A^* \lambda)' - B^* \lambda = 0$$

$A = \partial F / \partial \dot{x}$ nonsingular, $B = \partial F / \partial x$
Can use

$$(\lambda^* A)_{t=t_f} = 0$$

and therefore

$$\nabla_p G = \int_{t_0}^{t_f} (g_p - \lambda^* F_p)\; dt + (\lambda^* F_{\dot{x}})_{t=t_0}\, x_{0p}$$

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Hessenberg index-2 DAE

$$\begin{aligned} \dot{x}^d &= f^d(x^d, x^a, p) \\ 0 &= f^a(x^d, p) \end{aligned} \quad \Rightarrow \quad \begin{aligned} \dot{\lambda}^d &= -A^* \lambda^d - C^* \lambda^a - g^*_{x^d} \\ 0 &= -B^* \lambda^d - g^*_{x^a} \end{aligned}$$

Search for final conditions of the form $\lambda^d(t_f) = (C^* \xi)_{t=t_f}$

$$t = t_f \Rightarrow \begin{cases} \lambda^{d*} B = -g_{x^a} \Rightarrow \xi^* CB = -g_{x^a} \Rightarrow \xi^* = -g_{x^a}(CB)^{-1} \\ f^a(x^d, p) = 0 \rightarrow Cx^d_p = -f^a_p \Rightarrow \lambda^{d*} x^d_p = -xi^* f^a_p \end{cases}$$

$$\Rightarrow \lambda^{d*}(t_f) = -\left(g_{x^a}(CB)^{-1} C\right)_{t=t_f}$$

$$\Rightarrow \nabla_p G = \int_{t_0}^{t_f} \left(g_p + \lambda^{d*} f^d_p + \lambda^{a*} f^a_p\right) dt + \lambda^{d*}(t_0) x^d_{0p} + \left(g_{x^a}(CB)^{-1} f^a_p\right)_{t=t_f}$$

ASA implementation issues

CASC

Problem

Solution of the forward problem is needed in the backward integration phase ⇒ need predictable and compact storage of state variables for the solution of the adjoint system.

Solution: checkpointing

- Simulations are reproducible from each checkpoint
- Force Jacobian evaluation at checkpoints to avoid storing it
- Store solution (and possibly first derivative) at all intermediate steps between two consecutive checkpoints
- Interpolation options: cubic Hermite, variable-order polynomial

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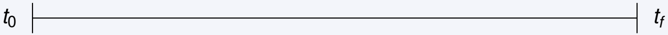
Checkpointing

Implementation

1. integrate forward step by step
2. dump checkpoint data after a given number of steps
3. continue until t_f.
4. evaluate final conditions for adjoint problem
5. store interpolation data on second forward pass
6. propagate adjoint variables backward in time
7. total cost: 2 forward passes + 1 backward pass



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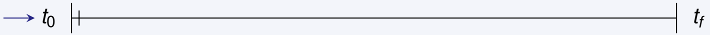

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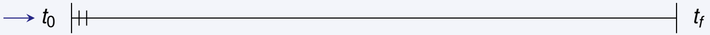

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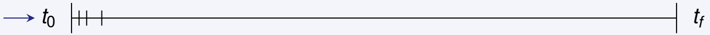

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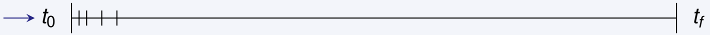

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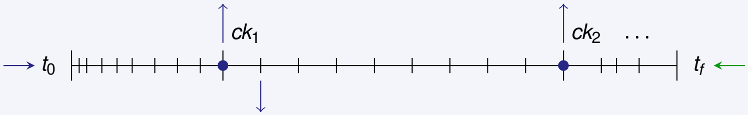

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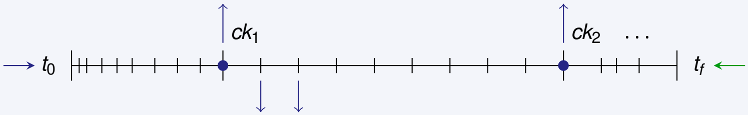

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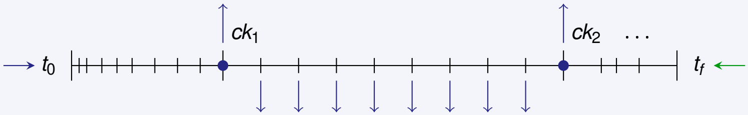

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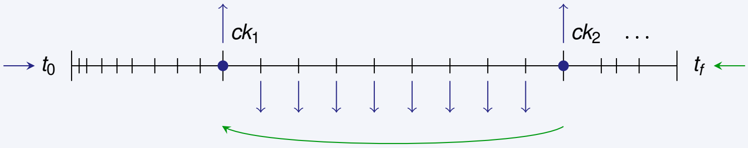

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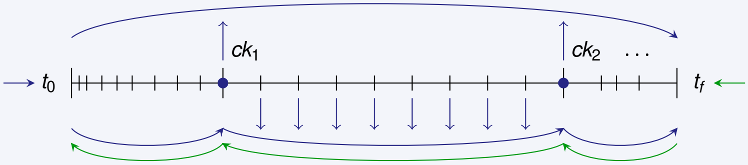
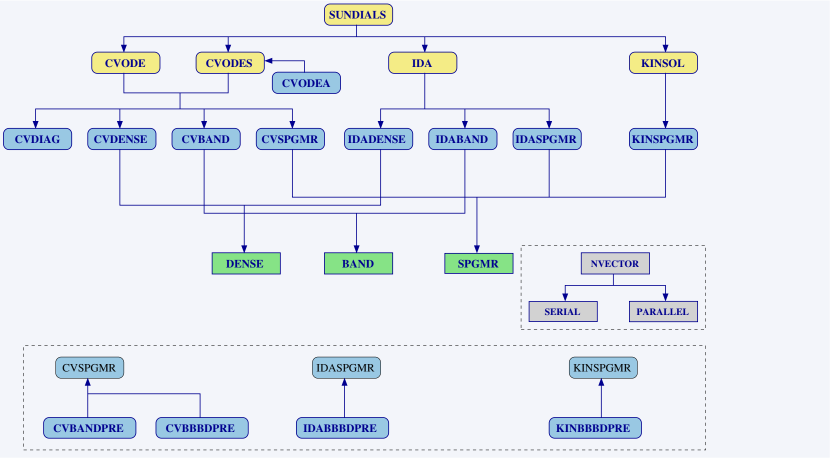
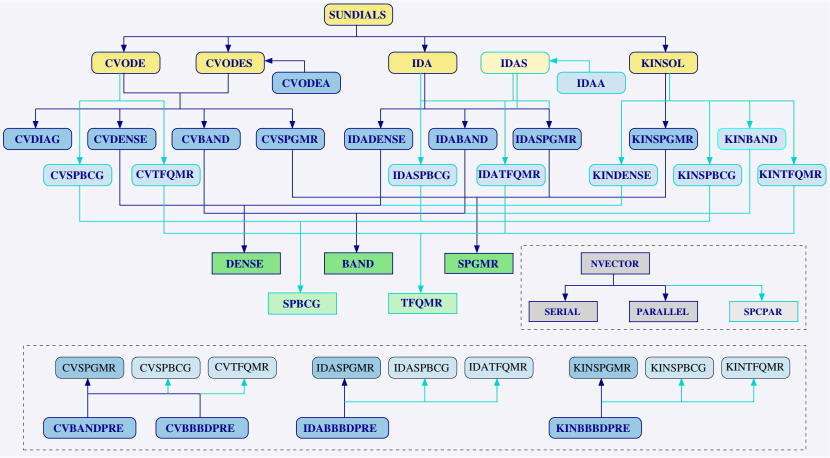


Outline

The SUNDIALS suite: v.2.1.1



The SUNDIALS suite: next release



IVP integration with CVODES

Main function

```
/* Set tolerances, initial time, etc. */
y = N_VNew_Serial(n);
/* Load I.C. into y */
cvode_mem = CVodeCreate(CV_BDF, CV_NEWTON);
flag = CVodeMalloc(cvode_mem, f, t0, y, CV_SS, rtol, atol);
flag = CVodeSetFdata(cvode_mem, my_data);
flag = CVDense(cvode_mem, n);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(cvode_mem, tout, y, &t, CV_NORMAL);
 /* Process solution y */
}
N_VDestroy_Serial(y);
CVodeFree(cvode_mem);
```

Required functions

- right-hand side
- quadrature integrand
- g-function

Optional functions

- Jacobian data
- preconditioner
- error weights

FSA with CVODES

Main function

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(...);
}
N_VDestroy*(y);
CVodeFree(cvode_mem);
```

FSA with CVODES

Main function (instrumented for FSA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
yS = N_VNewVectorArray*(...);
flag = CVodeSensMalloc(...);
flag = CVodeSetSens*(...);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(...);
 flag = CVodeGetSens(...);
}
N_VDestroy*(y);
N_VDestroyVectorArray*(...,yS);
CVodeFree(cvode_mem);
```

FSA with CVODES

CASC

Main function (instrumented for FSA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
yS = N_VNewVectorArray*(...);
flag = CVodeSensMalloc(...);
flag = CVodeSetSens*(...);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(...);
 flag = CVodeGetSens(...);
}
N_VDestroy*(y);
N_VDestroyVectorArray*(...,yS);
CVodeFree(cvode_mem);
```

FSA with CVODES

Main function (instrumented for FSA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
yS = N_VNewVectorArray*(...);
flag = CVodeSensMalloc(...);
flag = CVodeSetSens*(...);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(...);
 flag = CVodeGetSens(...);
}
N_VDestroy*(y);
N_VDestroyVectorArray*(...,yS);
CVodeFree(cvode_mem);
```

FSA with CVODES

Main function (instrumented for FSA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
yS = N_VNewVectorArray*(...);
flag = CVodeSensMalloc(...);
flag = CVodeSetSens*(...);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(...);
 flag = CVodeGetSens(...);
}
N_VDestroy*(y);
N_VDestroyVectorArray*(...,yS);
CVodeFree(cvode_mem);
```

FSA with CVODES

Main function (instrumented for FSA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
yS = N_VNewVectorArray*(...);
flag = CVodeSensMalloc(...);
flag = CVodeSetSens*(...);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(...);
 flag = CVodeGetSens(...);
}
N_VDestroy*(y);
N_VDestroyVectorArray*(...,yS);
CVodeFree(cvode_mem);
```

FSA with CVODES

Main function (instrumented for FSA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
yS = N_VNewVectorArray*(...);
flag = CVodeSensMalloc(...);
flag = CVodeSetSens*(...);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(...);
 flag = CVodeGetSens(...);
}
N_VDestroy*(y);
N_VDestroyVectorArray*(...,yS);
CVodeFree(cvode_mem);
```

FSA with CVODES

Main function (instrumented for FSA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
yS = N_VNewVectorArray*(...);
flag = CVodeSensMalloc(...);
flag = CVodeSetSens*(...);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(...);
 flag = CVodeGetSens(...);
}
N_VDestroy*(y);
N_VDestroyVectorArray*(...,yS);
CVodeFree(cvode_mem);
```

ASA with CVODES

Main function

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
for (iout=1; iout<= NOUT; iout++) {
 flag = CVode(...);
}
N_VDestroy*(y);
CVodeFree(cvode_mem);
```

ASA with CVODES

Main function (instrumented for ASA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
cvadj_mem = CVadjMalloc(...);
for (iout=1; iout<= NOUT; iout++) {
 /*flag = CVode(...);*/
 flag = CVodeF(...);
}
yB = N_VNew*(nB,...);
flag = CVodeCreateB(...);
flag = CVodeMallocB(...);
flag = CVodeSet*B(...);
flag = CVodeB(...);
N_VDestroy*(y);
CVodeFree(cvode_mem);
N_VDestroy*(yB);
CVadjFree(cvadj_mem);
```

ASA with CVODES

Main function (instrumented for ASA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
cvadj_mem = CVadjMalloc(...);
for (iout=1; iout<= NOUT; iout++) {
 /*flag = CVode(...);*/
 flag = CVodeF(...);
}
yB = N_VNew*(nB,...);
flag = CVodeCreateB(...);
flag = CVodeMallocB(...);
flag = CVodeSet*B(...);
flag = CVodeB(...);
N_VDestroy*(y);
CVodeFree(cvode_mem);
N_VDestroy*(yB);
CVadjFree(cvadj_mem);
```

ASA with CVODES

Main function (instrumented for ASA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
cvadj_mem = CVadjMalloc(...);
for (iout=1; iout<= NOUT; iout++) {
 /*flag = CVode(...);*/
 flag = CVodeF(...);
}
yB = N_VNew*(nB,...);
flag = CVodeCreateB(...);
flag = CVodeMallocB(...);
flag = CVodeSet*B(...);
flag = CVodeB(...);
N_VDestroy*(y);
CVodeFree(cvode_mem);
N_VDestroy*(yB);
CVadjFree(cvadj_mem);
```

ASA with CVODES

Main function (instrumented for ASA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
cvadj_mem = CVadjMalloc(...);
for (iout=1; iout<= NOUT; iout++) {
 /*flag = CVode(...);*/
 flag = CVodeF(...);
}
yB = N_VNew*(nB,...);
flag = CVodeCreateB(...);
flag = CVodeMallocB(...);
flag = CVodeSet*B(...);
flag = CVodeB(...);
N_VDestroy*(y);
CVodeFree(cvode_mem);
N_VDestroy*(yB);
CVadjFree(cvadj_mem);
```

ASA with CVODES

CASC

Main function (instrumented for ASA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
cvadj_mem = CVadjMalloc(...);
for (iout=1; iout<= NOUT; iout++) {
 /*flag = CVode(...);*/
 flag = CVodeF(...);
}
yB = N_VNew*(nB,...);
flag = CVodeCreateB(...);
flag = CVodeMallocB(...);
flag = CVodeSet*B(...);
flag = CVodeB(...);
N_VDestroy*(y);
CVodeFree(cvode_mem);
N_VDestroy*(yB);
CVadjFree(cvadj_mem);
```

ASA with CVODES

Main function (instrumented for ASA)

```
y = N_VNew*(n,...);
cvode_mem = CVodeCreate(...);
flag = CVodeMalloc(...);
flag = CVodeSet*(...);
cvadj_mem = CVadjMalloc(...);
for (iout=1; iout<= NOUT; iout++) {
 /*flag = CVode(...);*/
 flag = CVodeF(...);
}
yB = N_VNew*(nB,...);
flag = CVodeCreateB(...);
flag = CVodeMallocB(...);
flag = CVodeSet*B(...);
flag = CVodeB(...);
N_VDestroy*(y);
CVodeFree(cvode_mem);
N_VDestroy*(yB);
CVadjFree(cvadj_mem);
```

Some packages using SUNDIALS solvers

ARDRA Neutron and Radiation Transport
`http://www.llnl.gov/casc/Ardra/`

DELPHIN4 Coupled heat, moisture, air and salt transport
`http://www.bauklimatik-dresden.de/`

EMSO Environment for Modeling, Simulation, and Optimization
`http://vrtech.com.br/rps/emso.html`

magpar Parallel Finite Element Micromagnetics Package
`http://magnet.atp.tuwien.ac.at/scholz/magpar/`

Mathematica Wolfram Research
`http://www.wolfram.com/products/mathematica/index.html`

NEURON Empirically-based simulations of networks of neurons
`http://www.neuron.yale.edu/neuron/`

PETSc The Portable, Extensible Toolkit for Scientific Computation
`http://www-unix.mcs.anl.gov/petsc/`

SAMRAI Structured Adaptive Mesh Refinement Application Infrastructure
`http://www.llnl.gov/CASC/samrai/`

SBML Systems Biology Markup Language
`http://www.sbml.org/software/libsbml/`

Simulation applications

CASC

@LLNL

- **CVODE** is used in a 3D parallel tokamak turbulence model in LLNL's Magnetic Fusion Energy Division.
  Typical run: 7 unknowns on a 64x64x40 mesh, with 60 processors
- **KINSOL** with a hypre multigrid preconditioner is used in LLNL's Geosciences Division for an unsaturated porous media flow model.
  Fully scalable performance has been obtained on up to 225 processors on ASCI Blue.
- All solvers are being used to solve 3D neutral particle transport problems in CASC.
  Scalable performance obtained on up to 5800 processors on ASCI Red.
- Other applications: disease detection, astrophysics, magnetohydrodynamics, etc.

Other

- Many more in very different areas...

Sensitivity analysis applications

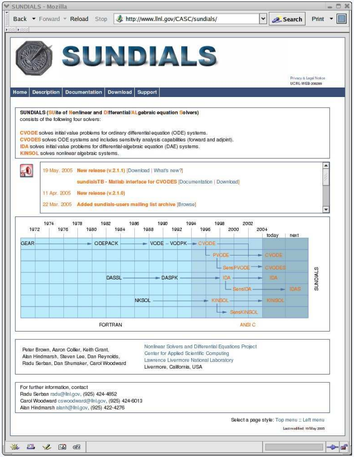
@LLNL

- Solution sensitivities in neutral particle transport applications
- Sensitivity analysis of groundwater simulations
- Sensitivity analysis of chemically reacting flows
- Sensitivity analysis of radiation transport (diffusion approximation)
- Inversion of large-scale time dependent PDEs (atmospheric releases).

Other

- Optimization of periodic adsorption processes (L.T. Biegler, CMU)
- Nonlinear model predictive control (A. Romanenko, Enginum)
- Controller design (Y. Cao, Cranfield U.)

www.llnl.gov/CASC/sundials



The SUNDIALS suite

- Open source, BSD license
- Complete documentation (HTML, PDF, PS)
- User support (mailing lists, Bugzilla bug tracking)
- (May 19, 2005): Matlab interface to **CVODES** and **KINSOL**

The SUNDIALS team

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Past contributors

Scott Cohen and Allan Taylor

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