The semi-Lagrangian semi-implicit technique of the ECMWF model

by Michail Diamantakis (room 2107; ext. 2402) michail.diamantakis@ecmwf.int



What do we want to achieve?

We want to build an <u>accurate</u> and <u>robust</u> global weather forecasting system at the <u>lowest possible cost</u>

- Role of numerical technique is central into achieving this goal
- Semi-Lagrangian (SL) semi-implicit (SI) technique can do it!
 - Unconditionally stable advection scheme having good phase speeds with little numerical dispersion
 - \rightarrow No CFL restriction in $\Delta t!$
 - Unconditional stability of semi-implicit technique
 - → No restriction in ∆t from integration of "fast forcing" terms such as gravity wave + acoustic terms



What is a semi-Lagrangian transport method?

- A numerical technique for solving transport problems which applies Lagrangian "thinking" on grid-point models when solving transport equations:
 - It is like a Lagrangian method: fluid parcels follow a Lagrangian trajectory
 - However, at each time-step a <u>parcel trajectory</u> always <u>terminates on a grid-point</u>. Mesh is not allowed to "depart" too much from its original form (constant resetting at every time-step).
 - It gradually evolved to current form from schemes introduced in the '50s, '60s and 70s (Wiin-Nielsen, Krishnamurti, Sawyer, Leith, Purnel)



History of semi-Lagrangian IFS

- IFS: Integrated Forecast System for medium range forecasts operating since 1979
- Until the beginning of 1991 IFS is a spectral Eulerian model on a full Gaussian grid at T106 horizontal resolution and 19 levels
 - ♦ An increase to T231 L31 resolution was planned
 - This upgrade required at least 12 x available CPU power
 - ♦ Funding was available for 4 x CPU increase ...
- Upgrade was made possible only due to switching to:
 - A semi-Lagrangian scheme on a reduced Gaussian grid
 - The new model was 6 x faster!

Basic concepts: the departure point

Advection equation without forcing:

$$\frac{D\phi}{Dt} \equiv \frac{\partial\phi}{\partial t} + V \cdot \nabla \phi = 0, \quad V = (u, v, w)$$

At time t parcel is at d and at t + Δt arrives at a grid-point $\phi_d^t = V \phi_a^{t+\Delta t}$
$$\int_{t}^{t+\Delta t} \frac{D\phi}{Dt} Dt = 0 \Rightarrow \phi^{t+\Delta t} = \phi_d^t$$

parcel trajectory in Δt
d: departure point (d.p.) a : arrival point

Finding the "departure point" is an essential part of the technique:

- Solution at t+∆t is obtained by interpolating the available (defined at time t) grid-point *φ*-values at the d.p.
- ♦ Nonlinear term V · ∇ \u03c6 is absorbed by the Lagrangian derivative: nonlinear advection turned to interpolation!

Semi-Lagrangian semi-implicit technique in IFS Slide 5



A simple Semi-Lagrangian algorithm

Solve

$$\frac{D\phi}{Dt} = 0, \quad V = (u, v, w).$$

At the beginning of each step field values ϕ_j are available on the model grid. To compute next time step solution:

- 1. First compute departure point (d.p.) location, e.g. for simple case with constant wind V_0 : $x_{d,j} = x_j V_0 \Delta t$
- 2. Using field values at nearest points surrounding $X_{d,j}$ interpolate field ϕ_j^t to obtain solution at future time $t + \Delta t$ i.e.

$$\phi_j^{t+\Delta t} = \phi_d^t \equiv I(\phi_j^t) \Big|_{x_d}, I = \text{ interpolation operator}$$

ECM

Accurate calculation of d.p. and an accurate interpolation scheme are essential!

Stability in one dimension



Departure to arrival pt distance (displacement): $x_j - x_d = u_0 \Delta t = (p + \alpha) \Delta x$ p: integer

Assuming linear interpolation $\phi_j^{n+1} = \phi_d^n = (1 - \alpha)\phi_{j-p}^n + \alpha\phi_{j-p-1}^n$, $\alpha = \frac{x_{j-p} - x_d}{\Delta x}$ conduct Von Neuman stability analysis:

$$\phi_j^n = \phi_0 \lambda^n e^{ikj\Delta x} \longrightarrow \lambda = \left[1 - \alpha (1 - e^{-ik\Delta x})\right] e^{-ipk\Delta x}$$

Amplification factor: $|\lambda|^2 = 1 - 2\alpha(1 - \alpha)[1 - \cos(k\Delta x)]$

 $|\lambda| \le 1$ if $0 \le \alpha \le 1$ (interpolation from two nearest points)

NOTE: when $p=0 \Rightarrow \alpha$ is the CFL number \Rightarrow SL with linear interpolation is essentially Eulerian upstream differencing!

Linear interpolation = damping! Semi-Lagrangian semi-implicit technique in IFS Slide 7

How to find d.p. in SL NWP models

In atmospheric flows wind field changes in space and time

To find departure points, solve equation:

 $\frac{Dr}{Dt} = V(r,t)$ where r, V the position and wind vector

along a trajectory. Second order mid-point rule is often used:

$$\int_{t}^{t+\Delta t} Dr = \int_{t}^{t+\Delta t} V(r,t)Dt \Rightarrow r_{a}^{t+\Delta t} - r_{d}^{t} = \int_{t}^{t+\Delta t} V(r,t)dt \approx \Delta t V(r_{M}, t + \Delta t/2)$$
t-extrapolation needed: $V(t+\Delta t/2) = \frac{3}{2}V(t) - \frac{1}{2}V(t-\Delta t)$ Trajectory midpoint
For 3-time
level scheme: $\frac{r_{a}^{t+\Delta t} - r_{d}^{t-\Delta t}}{2\Delta t} = V(r,t) \Rightarrow r_{a}^{t+\Delta t} - r_{d}^{t-\Delta t} = \int_{t}^{t+\Delta t} Udt \approx \Delta t V(r_{M},t)$
No t-extrapolation
but expensive

ECM

eparture point is computed iteratively

Iterative scheme for computing d.p.

- Consider two time-level (TL) scheme and assume that during a time-step parcels follow straight lines (great circle) trajectories
 - Define displacement vector:

$$d \equiv r_a - r_d \Longrightarrow r_M \equiv \frac{r_a + r_d}{2} = r_a - \frac{d}{2}$$

$$r_a \equiv r^{t+\Delta t}$$

is known! Arrival points are
always grid points!

• Iterate discretized trajectory equation $\frac{Dr}{Dt} = V(r,t)$

$$d^{(0)} = 0$$

$$d^{(k)} = \Delta t V \left(r_a - \frac{d^{(k-1)}}{2}, t + \frac{\Delta t}{2} \right), \quad k = 1, 2, ... K$$
Interpolate V at r-d^(k-1)/2 (use linear interpolation)
Extrapolate V at t+ $\Delta t/2$
normally K=2

Smolarkiewicz & Pudikiewicz (J. Atmos. Sci.1992): Convergence requires satisfaction of a Lipschitz condition (parcels trajectories do not cross): $\Delta t |\partial V / \partial r| < 1$ Doesn't depend on mesh size and less restrictive than CFL for atmospheric flows

Semi-Lagrangian semi-implicit technique in IFS Slide 9

Time extrapolated winds and stability

When computing d.p extrapolating V at t+ $\Delta t/2$ can be a source of weak instability Cordero et al (QJRMS, 2005). Solutions:

- a. Iterative (expensive) approach:
 - 1. Time-step dynamics once to obtain V(t+ Δ t) estimate (predictor)
 - 2. Time-step again BUT now use predictor to interpolate at t+ $\Delta t/2$: V(t+ $\Delta t/2$)=[V(t)+V(t+ Δt)]/2
- b. Use Stable Extrapolating Two Time-Level Semi-Lagrangian (SETTLS) scheme (low cost) by Hortal (QJRMS, 2002)



Standard extrapolation

T forecast 200 hPa (from 1997/01/04)





Semi-Lagrangian semi-implicit technique in IFS Slide 10

SETTLS for computing departure points

Taylor expansion to second order:

$$r_a(t + \Delta t) = r_d(t) + \Delta t \cdot \left(\frac{Dr}{Dt}\right)_d^t + \frac{\Delta t^2}{2} \cdot \left(\frac{D^2 r}{Dt^2}\right)_{AV}$$

AV: average value along SL trajectory

ECMW

$$\left(\frac{Dr}{Dt}\right)_{d}^{t} = V_{d}(t)$$
 and $\left(\frac{D^{2}r}{Dt^{2}}\right)_{AV} = \left(\frac{DV}{Dt}\right)_{AV} \approx \frac{V_{a}(t) - V_{d}(t - \Delta t)}{\Delta t}$

Hence,

$$r_a(t + \Delta t) \approx r_d(t) + \frac{\Delta t}{2} \cdot \left(V_a(t) + \left\{2V(t) - V(t - \Delta t)\right\}_d\right)$$

Therefore d.p. can be computed by iterative sequence:

$$r_d^{(k)} = r_a - \frac{\Delta t}{2} \cdot \left(V_a(t) + \left\{ 2V(t) - V(t - \Delta t) \right\} \Big|_{r_d^{(k-1)}} \right) k = 1, 2, \dots$$

Interpolate at $r_d^{(k-1)}$

SETTLS extrapolation weaknesses

- Noise in upper stratosphere often occurring in "Sudden Stratospheric Warming" events (model doesn't predict accurately the warming event)
- A solution: use hybrid SETTLS/non-extrapolating scheme in vertical (see ecmwf newsletter No.141 Autumn 2014, M. Diamantakis)



ECMW

Interpolation in the IFS semi-Lagrangian scheme

Remember that there are two important steps in SL algorithm:

- 1. Compute departure point (trajectory calculation)
- 2. Interpolate advected field to d.p. to obtain: $\varphi^{t+\Delta t} = \varphi_d^t$ Interpolation must use (for stability) neighbouring to d.p. gridpoints ECMWF model uses <u>quasi-monotone</u> <u>quasi-cubic</u> Lagrange interpolation

Cubic Lagrange interpolation:
$$\varphi(x) = \sum_{i=1}^{4} C_i(x)\varphi_i$$
, $C_i(x) = \frac{\prod_{k\neq i}^{4} (x - x_k)}{\prod_{k\neq i}^{4} (x_i - x_k)}$



Number of 1D cubic interpolations in 2D: 5 =>3D: 21 (64pt stencil)

To save computations: *cubic interpolation only for nearest neighbour rows, linear interpolation remaining i.e. "quasi-cubic interpolation"*=> 7**cubic*+10**linear in 3D* (32 pt stencil)



X

Shape-preserving (locally monotonic) interpolation

• Creation of "artificial" maxima /minima







SL advection on the sphere

```
Temperton et al (QJRMS 2001)
```

Momentum eq. is discretized in vector form (a vector is continuous across the

poles, components are not!)

Trajectories are arcs of great circles if constant (angular) velocity is assumed for the duration of a time step.



To transport a vector use local reference system and apply rotation matrix from D to A to take into account earth's curvature
Interpolations at D are done for u & v components of the velocity vector relative to the system of reference local at D.

$$\begin{pmatrix} u_A \\ v_A \end{pmatrix} = \Re \begin{pmatrix} u_D \\ v_D \end{pmatrix}$$
Rotation

matrix

Slide 15



Trajectory calculation Semi-Lagrangian semi-implicit technique in IFS

SL issues and practices to be aware

- For a p-th order interpolation scheme global truncation error in linear advection (constant wind) case is $O((\Delta x)^{p+1}/\Delta t)$:
 - i.e. smaller timestep doesn't necessarily improve accuracy!
 (however, improves accuracy in the calculation of d.p.)
- When computing the d.p. usually 2-3 iterations are sufficient (Mac Donald, MWR 1987). However, if time-step is very long 2 may not be enough everywhere ...
- Cheap linear interpolation works well for the wind component interpolations in d.p. iterations (Temperton & Staniforth, QJRMS 1987)
- For SL models cubic Lagrange with quasi-monotone limiter is a standard option for interpolating fields to d.p.

ECM

Applying SLSI time stepping to NWP eqns

We want to solve a nonlinear system of m-prognostic equations:

$$\frac{DX}{Dt} = F(X), X = (X_1, X_2, ..., X_m)$$
 e.g. X=(u,v,T,p,q,...)

 Integrate along SL trajectory and approximate (using 2nd order trapezoidal scheme): Implicit and nonlinear coupling.

$$\mathbf{X}_{a}^{t+\Delta t} - \mathbf{X}_{d}^{t} = \int_{t}^{t+\Delta t} \mathbf{F}(\mathbf{X}) dt \Longrightarrow \mathbf{X}_{a}^{t+\Delta t} - \mathbf{X}_{d}^{t} = \frac{\Delta t}{2} \left(\mathbf{F}_{d}^{t} + \mathbf{F}_{a}^{t+\Delta t} \right)$$

♦ Linearize fast nonlinear terms. Let L contain linearized fast terms + linear RHS terms e.g. $L_{PGT} \equiv R_d T_{ref} \ln p_s \approx R_d T_v \nabla_h \ln p$

Choose L, then $N = F - L \Rightarrow F = N + L$

nonlinear "slow" terms: these "Fast linearized" (GW/acoustic) terms will be integrated explicitly

Applying SLSI to NWP eqns (II)

Two-time-level, 2nd order IFS discretization (Temperton et al, QJRMS 2001):



 $N^{t+\Delta t/2}$ can be obtained "explicitly" using one of the two extrapolation schemes discussed:



ECMV

2nd order accurate formula (can be verified by Taylor expansion)

Assembling all equations: Helmholtz solver

- We have m prognostic equations discretized implicitly and N grid points \Rightarrow implicit $mN \ge mN$ system (expensive!)
 - Manipulating the equations, we can eliminate the variables to derive a single N x N elliptic (Helmholtz) equation. Once this is solved all prognostic variables can be updated through "back-substitution".
 - ♦ IFS: Helmholtz equation in terms of horizontal divergence
 - A constant coefficient system. Using spherical Harmonics properties can be solved very accurately and efficiently!
 - → Cheap solver + large ∆t (cf. unconditional stability of SL advection) explains why IFS is such an efficient model



2-TL SLSI integration of IFS hydrostatic PE set

$$\frac{D\mathbf{V}_{h}}{Dt} + f\mathbf{k} \times \mathbf{V}_{h} + \nabla_{h}\Phi + R_{d}T_{v}\nabla_{h}\ln p = P_{v}$$

$$\frac{DT}{Dt} - \frac{\kappa T_{v}\omega}{(1 + (\delta - 1)q)p} = P_{T}, \qquad \frac{Dq}{Dt} = P_{q}$$

$$\frac{D}{Dt}(\ln p_{s}) = \mathbf{V}_{h} \cdot \nabla_{h}(\ln p_{s}) - \frac{1}{p_{s}}\int_{0}^{1}\nabla_{h} \cdot (\mathbf{V}_{h}\frac{\partial p}{\partial \eta})d\eta$$

$$\Phi = \Phi_{s} - \int_{1}^{\eta}R_{d}T_{v}\frac{\partial}{\partial \eta}(\ln p)d\eta$$

$$P = \Phi_{s} - \int_{1}^{\eta}R_{d}T_{v}\frac{\partial}{\partial \eta}(\ln p)d\eta$$

$$P = \Phi_{s} - \int_{0}^{\eta}R_{d}T_{v}\frac{\partial}{\partial \eta}(\ln p)d\eta$$

$$P = \Phi_{s} - \int_{0}^{\eta}\nabla_{s}(\nabla_{s}(\nabla_{s}(\ln p_{s}) - \frac{1}{\rho_{s}}\int_{0}^{\eta}\nabla_{s}(\nabla_{s}(\ln p_{s}) - \frac{1}{\rho_{s}}\int_{0}^{\eta}\nabla$$

Deriving Helmholtz equation (part I)

Here for simplicity assume dry dynamics $(T=T_v)$. Also assume that Coriolis are incorporated in V_h i.e. advect $X = V_h + 2\Omega \times r$ Having defined L, N we write the 2nd order semi-implicit time discretization as:

$$\frac{X^{t+\Delta t} - X_d^t}{\Delta t} = 0.5(L_d^t + L^{t+\Delta t}) + 0.5(N_d^{t+\Delta t/2} + N^{t+\Delta t/2})$$

$$X^{t+\Delta t} - 0.5\Delta t L_t^{t+\Delta t} = \underbrace{X_d^t + 0.5\Delta t L_d^t + 0.5\Delta t (N_d^{t+\Delta t/2} + N^{t+\Delta t/2})}_{\equiv X^*(known part)}$$

$$\mathbf{V}_h^{t+\Delta t} - 0.5\Delta t \mathbf{L}_V^{t+\Delta t} = \mathbf{V}^*$$

$$T^{t+\Delta t} - 0.5\Delta t L_T^{t+\Delta t} = T^*$$

$$\ln p_s^{t+\Delta t} - 0.5\Delta t L_p^{t+\Delta t} = P^*$$

$$\mathbf{D}^{t+\Delta t} + 0.5\Delta t \underbrace{\tau}_D^{t+\Delta t} = T^*$$

$$\ln p_s^{t+\Delta t} + 0.5\Delta t \underbrace{\tau}_D^{t+\Delta t} = P^*$$

$$\mathbf{L}_{V} \equiv -\nabla_{h} (\underbrace{\gamma}_{E} T + R_{d} T_{ref} \ln p_{s}), \quad L_{T} = -\underbrace{\tau}_{E} D, \quad L_{p} = -\underbrace{\nu}_{E} D$$

 T_{ref} : constant temperature reference profile

 $\underline{\gamma}, \underline{\tau}, \underline{\nu}$: operators defined in Ritchie et al MWR vol123, 1995

D: horizontal divergence

Semi-Lagrangian semi-implicit technique in IFS Slide 21



Deriving and solving Helmholtz equation

Eliminate T, ln p_s to derive a Helmholtz equation wrt to D:

$$\left(1 - \alpha^{2} \Delta t^{2} (\underbrace{\gamma \tau}_{\underline{z}} + R_{d} T_{ref} \underbrace{\nu}_{\underline{z}}) \nabla_{h}^{2} \right) D^{t + \Delta t} = D^{*} - \alpha \Delta t \nabla_{h}^{2} (\underbrace{\gamma \tau}_{\underline{z}} + R_{d} T_{ref} P^{*}) \quad a=0.5$$

(off-centring i.e. α -value >0.5 increases damping. It is an option in IFS code but is not used operationally – not essential in IFS and reduces accuracy)

Define:
$$\underline{\Gamma} \equiv \alpha^2 \Delta t^2 \left(\underbrace{\gamma \tau}_{\underline{\tau}} + R_d T_r \underbrace{\nu}_{\underline{t}} \right), \Re = D^* - \alpha \Delta t \nabla_h^2 \left(\underbrace{\gamma T}_{\underline{\tau}} + R_d T_r P^* \right)$$
$$\left(\underbrace{I}_{\underline{t}} - \underline{\Gamma} \nabla_h^2 \right) D^{t + \Delta t} = \Re$$

Decouple equations by diagonalizing Γ , transform in spectral space

$$\underline{\underline{\Gamma}} = S^{-1}\underline{\underline{\Lambda}}S, \quad \widetilde{D}^{t+\Delta t} = SD^{t+\Delta t}, \quad \widetilde{\mathfrak{R}} = S\mathfrak{R} \Longrightarrow \left(\underline{\underline{I}} - \underline{\underline{\Lambda}}\nabla_{h}^{2}\right)\widetilde{D}^{t+\Delta t} = \widetilde{\mathfrak{R}}$$

$$\left(1 - \lambda_i \nabla_h^2\right) \widetilde{D}_i^{t+\Delta t} = \widetilde{\mathfrak{R}}_i, \ 1 \le i \le N_{Lev}, \ \ \widetilde{D}_i \equiv \widetilde{D}_{n,i}^m$$

$$\nabla^2 \widetilde{D}_{n,i}^m = -\frac{n(n+1)}{r_0} \widetilde{D}_{n,i}^m \longrightarrow \left(1 + \lambda_i \frac{n(n+1)}{r_0^2}\right) \widetilde{D}_{n,i}^{m}^{t+\Delta t} = \widetilde{\mathfrak{R}}_{n,i}^m$$

- 1 trivial eqn/lev
- Back-substitute to update remaining fields



Issues in SI time stepping to be aware

- SI time stepping as implemented in IFS and other operational models is not strictly unconditionally stable
 - extrapolations are a source of instability. Therefore,
 - need to carefully consider how to split the right hand side to fast linear (L) and slow nonlinear (N) terms
 - In IFS SETTLS extrapolation of nonlinear terms is used
- Iterative approach can eliminate such stability problems
 - ♦ Available in IFS (ICI: Iterative Centred Implicit)
 - ◆ Iterative approach works like predictor-corrector: no need to extrapolate at the corrector stage as a good predictor for the atmospheric state at t+∆t exists. However, expensive!

ECI



Limitations of the SLSI approach

Not formally conserving

- In long integrations mass drifts and needs to be "fixed"
- In IFS and most SL models mass fixers are used for tracers and air mass in long simulations (GMD 2014, Diamantakis & Flemming)
- Inherently mass conserving SL schemes do exist but haven't been used into operations so far (expensive, issues with complex terrain)
- Scalability issues at convection permitting resolution:
 - IFS: high communication cost of transpositions (gridpoint -> spectral -> gridpoint)

ECN

• UKMO: high cost Helmholtz solver on lat/lon grid

Semi-Lagrangian semi-implicit technique in IFS Slide 24

Inherently conserving SL schemes

- Air mass / tracer local and global mass conservation
- Essentially, they are finite-volume SL methods (e.g. UK Met Office SLICE-ENDGAME). Ensuring that:
 - mass in dep volume=mass in arrival (grid) volume



However, for NWP, these are costly alternatives to standard gridpoint SLSI. They can outperform conservative Eulerian finitevolume methods when many tracers are advected (e.g. climate models), an example is CSLAM (Lauritzen et al, JCP 2010)

EC

Some references

- Staniforth and Cote (MWR 1990) review paper: "Semi Lagrangian schemes for Atmospheric models"
- Ritchie et al (MWR 1995): "Implementation of the Semi-Lagrangian Method in a High-Resolution version ..."
- Temperton, Hortal, Simmons (QJRMS 2001): "A two-timelevel semi-Lagrangian global spectral model"
- Hortal (QJRMS 2002): "The development and testing of a new two-time level semi-Lagrangian scheme (SETTLS) in the ECMWF forecast model"

ECM

- Dale Durran's book: "Numerical methods for Wave Equations in Geophysical Fluid Dynamics" (1999)
- Training course notes & references in slides



Thank you for your attention!

