

NOE Optimization

January 2, 2017 11:12 AM

Continues 2016-11/Figuring out NOE; excerpt from NOEOptimizationBase.nb.

NOE-It

```
Ri,j+ := E[1, Log[ti] lj, ei fj, ei li fj + li lj + ei2 fj2 / 4];  
Ri,j- := E[1, -Log[ti] lj, -ti-1 ei fj, -li lj + ti-1 ei lj fj - ti-2 ei2 fj2 / 4];  
(uri := E[ti-1/2, 0, 0, li ti-2]; nri := E[ti1/2, 0, 0, -li ti2];)
```

```
DPx→Dα, y→Dβ[P-][f-] := (* means P[∂α, ∂β][f] *)  
PPDP@Total[CoefficientRules[P, {x, y}] /. ({m-, n-} → c-) ⇒ c D[f, {α, m}, {β, n}]]
```

```
CF[E[ω-, L-, Q-, P-]] :=  
PPCF@E[Expand@Together@ω, Expand@Together@L, Expand@Together@Q,  
Expand@PPTogether4P@Together@P];
```

```
E /: E[ω1-, L1-, Q1-, P1-] E[ω2-, L2-, Q2-, P2-] :=  
CF@E[ω1 ω2, L1 + L2, ω2 Q1 + ω1 Q2, ω24 P1 + ω14 P2];
```

```
Δ[k-] := ((tk - 1) (2 (α β + δ μ)2 - α2 β2) - 4 ek lk fk δ2 μ2 -  
δ (1 + μ) (fk2 α2 + ek2 β2) - ek2 fk2 δ3 (1 + 3 μ) -  
2 (α β + 2 δ μ + ek fk δ2 (1 + 2 μ) + 2 lk δ μ2) (fk α + ek β) -  
4 (lk μ2 + ek fk δ (1 + μ)) (α β + δ μ)) (1 + tk) / 4;
```

```
Nfi ej → k-[E[ω-, L-, Q-, P-]] := PPNfe@With[{q = ((1 - tk) α β + β ek + δ ek fk + α fk) / μ}, CF[  
E[μ ω, L, μ ω q + μ (Q / fi | ej → 0), μ4 (DPfi → Dα, ej → Dβ[P][eq] /. e- → 1) + ω4 Δ[k]]] /.  
μ → 1 + (tk - 1) δ / {α → ω-1 (∂fi Q / ej → 0), β → ω-1 (∂ej Q / fi → 0),  
δ → ω-1 ∂fi, ej Q}]]];
```

Break in 5 pieces!

```
Nlj (x:e|f) i → k-[E[ω-, L-, Q-, P-]] := PPNlx@With[{q = eγ β xk + γ lk}, CF[  
E[ω, γ lk + (L / lj → 0), ω eγ β xk + (Q / xi → 0), e-q DPlj → Dγ, xi → Dβ[P][eq]]] /.  
{γ → ∂lj L, β → ω-1 ∂xi Q}]]];
```

```
mi,j → k-[Z-E] := PPm@Module[{x, z},  
CF[(Z // Nfi ej → x // Nli ex → x // Nfx lj → x) / . Z-i|j|x → Zk]]
```