Challenges with the currently (correctly) implemented NEB-method. Should ASE revert to the original more robust NEB-formulation with springs?

Bjørk Hammer  
Aarhus University, Denmark

- **Motivation**: often seen that finding saddle points with ASE is challenging.
- **Objective**: assure easy and simple access to saddle point search with ASE
- **Means**:  
  - Illustrate pit-falls of current NEB implementation  
  - Illustrate robustness of old NEB implementation
Challenges with the currently (correctly)

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Activity of fully oxygen covered stepped metal surfaces

Z. Sljivancanin and BH, Phys Rev B 81, 121413(R) (2010)
Ethanol dissociation

Model system: Initial configuration
Model system: Final configuration
Success 1: Linear interpolation, many images
Success 1: standard ASE-NEB, many images
More typical: Few images.
After some iterations: a local minimum

25 iterations
After some iterations: a local minimum
Identifying the local minimum along the path
Identifying the local minimum along the path
Success 2: Climbing NEB
Success 2: Climbing NEB
Failure 1: Continued NEB
Failure 1: Two new local minima
Failure 1: Two new local minima
Failure 1: Finding the first local minimum
Failure 1: Finding the first local minimum
Failure 1: Finding the 2nd local minimum
Failure 1: Finding the 2nd local minimum
Failure 1: NEB between new minima
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Failure 1: NEB between new minima
Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points

Graeme Henkelman\textsuperscript{a)} and Hannes Jónsson\textsuperscript{b)}
Department of Chemistry, Box 351700, University of Washington

\[ \tau_i = \begin{cases} 
\tau_i^+ & \text{if } V_{i+1} > V_i > V_{i-1} \\
\tau_i^- & \text{if } V_{i+1} < V_i < V_{i-1} 
\end{cases} \]

where

\[ \tau_i^+ = R_{i+1} - R_i, \quad \text{and} \quad \tau_i^- = R_i - R_{i-1}, \]

\[ F_i^s = k \left[ (R_{i+1} - R_i) - (R_i - R_{i-1}) \right] \cdot \hat{\tau}_i \]

\[ F_i^s = k (|R_{i+1} - R_i| - |R_i - R_{i-1}|) \hat{\tau}_i \]
ASE version / neb.py code

```python
imax = 1 + np.argsort(energies)[-1]
self.emax = energies[imax - 1]

tangent1 = images[1].get_positions() - images[0].get_positions()
for i in range(1, self.nimages - 1):
    tangent2 = (images[i + 1].get_positions() - images[i].get_positions())
    if i < imax:
        tangent = tangent2
    elif i > imax:
        tangent = tangent1
    else:
        tangent = tangent1 + tangent2

    tt = np.vdot(tangent, tangent)
    f = forces[i - 1]
    ft = np.vdot(f, tangent)
    if i == imax and self.climb:
        f = 2 * ft / tt * tangent
    else:
        f = ft / tt * tangent
    f = np.vdot(tangent1 * self.k[i - 1] -
               tangent2 * self.k[i], tangent) / tt * tangent

tangent1 = tangent2
```

\[ \mathbf{F}_i \| = k[(\mathbf{R}_{i+1} - \mathbf{R}_i) - (\mathbf{R}_i - \mathbf{R}_{i-1})] \cdot \hat{\mathbf{r}}_i \hat{\mathbf{r}}_i \]
Solution: spring-NEB
Solution: spring-NEB
Solution: spring-NEB
Solution: spring-NEB
Solution: spring-NEB
Solution: spring-NEB
Solution: spring-NEB
Solution: spring-NEB + climbing-NEB
Solution: spring-NEB + climbing-NEB
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- **Observation:** finding saddle points with ASE is challenging.

- **Problem:** images may drift apart with:

  \[ F_i^S = k ( |R_{i+1} - R_i| - |R_i - R_{i-1}| ) \hat{\tau}_i \]

- **Solution:** reintroduce springs?