### Levi-Civita formulation

2D system:  $u_1, u_2$ 

$$R_1 = u_1^2 - u_2^2 R_2 = 2u_1u_2$$

Transformation

$$\mathbf{R} = \mathcal{L}(\mathbf{u})\mathbf{u}$$

Levi-Civita [1920] matrix

$$\mathcal{L}(\mathbf{u}) = \begin{bmatrix} u_1 & -u_2 \\ u_2 & u_1 \end{bmatrix} \qquad \Rightarrow \ R = u_1^2 + u_2^2$$

Definition  $\dot{\mathbf{R}}^2 = \dot{\mathbf{R}}^T \cdot \dot{\mathbf{R}}$  with  $\mathbf{R}' = 2\mathcal{L}(\mathbf{u})\mathbf{u}'$  and  $\dot{R} = R'/R$  $\dot{\mathbf{R}} = 2\mathcal{L}(\mathbf{u})\mathbf{u}'/R$ 

$$\dot{\mathbf{R}}^T = 2\mathbf{u}'\mathcal{L}^T(\mathbf{u})/R$$
 and  $\mathcal{L}^T(\mathbf{u})\mathcal{L}(\mathbf{u}) = R\mathbf{I}$  give  $\dot{\mathbf{R}}^T \cdot \dot{\mathbf{R}} = 4\mathbf{u}' \cdot \mathbf{u}'/R$ 

Final equation of motion, with  $\mathbf{u} \cdot \mathbf{u} = R$ 

$$\mathbf{u}'' = \frac{1}{2}h\mathbf{u} + \frac{1}{2}R\mathcal{L}^T(\mathbf{u})\mathbf{F}_{kl}$$

Binding energy per unit reduced mass

$$h = [(2\mathbf{u}' \cdot \mathbf{u}' - (m_k + m_l)]/R$$

Rate of change from  $\dot{\mathbf{R}} \cdot \ddot{\mathbf{R}}$ 

$$\frac{d}{dt} \left[ \frac{1}{2} \dot{\mathbf{R}}^2 - \frac{(m_k + m_l)}{R} \right] = \dot{\mathbf{R}} \cdot \mathbf{F}_{kl}$$

Conversion by  $h' = \mathbf{R}' \cdot \mathbf{F}_{kl}$  and  $\hat{\mathbf{R}}$ 

$$h' = 2\mathbf{u}' \cdot \mathcal{L}^T(\mathbf{u})\mathbf{F}_{kl}$$

#### KS formulation

2D system:  $u_1, u_2$ 

$$R_1 = u_1^2 - u_2^2 R_2 = 2u_1u_2$$

Transformation

$$\mathbf{R} = \mathcal{L}(\mathbf{u})\mathbf{u}$$

Levi-Civita [1920] matrix

$$\mathcal{L}(\mathbf{u}) = \begin{bmatrix} u_1 & -u_2 \\ u_2 & u_1 \end{bmatrix} \qquad \Rightarrow \ R = u_1^2 + u_2^2$$

Matrix properties (Stiefel & Scheifele 1970)

$$\mathcal{L}^{T}(\mathbf{u})\mathcal{L}(\mathbf{u}) = R\mathbf{I}$$

$$\mathcal{L}'(\mathbf{u}) = \mathcal{L}(\mathbf{u}')$$

$$\mathcal{L}(\mathbf{u})\mathbf{v} = \mathcal{L}(\mathbf{v})\mathbf{u}$$

$$\mathbf{u} \cdot \mathbf{u}\mathcal{L}(\mathbf{v})\mathbf{v} - 2\mathbf{u} \cdot \mathbf{v}\mathcal{L}(\mathbf{u})\mathbf{v} + \mathbf{v} \cdot \mathbf{v}\mathcal{L}(\mathbf{u})\mathbf{u} = 0$$

Second & third properties give

$$\mathbf{R}' = 2\mathcal{L}(\mathbf{u})\mathbf{u}'$$

From  $\mathcal{L}'(\mathbf{u}) = \mathcal{L}(\mathbf{u}')$ 

$$\mathbf{R''} = 2\mathcal{L}(\mathbf{u})\mathbf{u''} + 2\mathcal{L}(\mathbf{u'})\mathbf{u'}$$

Substituting  $\mathbf{R}, \mathbf{R}', R' = 2\mathbf{u}' \cdot \mathbf{u}$  and n = 1 in smoothed  $\mathbf{R}''$ 

$$2\mathbf{u} \cdot \mathbf{u} \mathcal{L}(\mathbf{u}) \mathbf{u}'' + 2\mathbf{u} \cdot \mathbf{u} \mathcal{L}(\mathbf{u}') \mathbf{u}' - 4\mathbf{u} \cdot \mathbf{u}' \mathcal{L}(\mathbf{u}) \mathbf{u}' + (m_k + m_l) \mathcal{L}(\mathbf{u}) \mathbf{u} = (\mathbf{u} \cdot \mathbf{u})^3 \mathbf{F}_{kl}$$

Simplification by fourth property

$$2\mathbf{u} \cdot \mathbf{u} \mathcal{L}(\mathbf{u}) \mathbf{u}'' - 2\mathbf{u}' \cdot \mathbf{u}' \mathcal{L}(\mathbf{u}) \mathbf{u} + (m_k + m_l) \mathcal{L}(\mathbf{u}) \mathbf{u} = (\mathbf{u} \cdot \mathbf{u})^3 \mathbf{F}_{kl}$$

Multiply by  $\mathcal{L}^{-1}(\mathbf{u})$  and first property

$$\mathbf{u}'' + \{[(m_k + m_l) - 2\mathbf{u}' \cdot \mathbf{u}']/2\mathbf{u} \cdot \mathbf{u}\}\mathbf{u} = \frac{1}{2}\mathbf{u} \cdot \mathbf{u}\mathcal{L}^T(\mathbf{u})\mathbf{F}_{kl}$$

Definition  $\dot{\mathbf{R}}^2 = \dot{\mathbf{R}}^T \cdot \dot{\mathbf{R}}$  with  $\mathbf{R}'$  and  $\dot{R} = R'/R$ 

$$\dot{\mathbf{R}} = 2\mathcal{L}(\mathbf{u})\mathbf{u}'/R$$

 $\dot{\mathbf{R}}^T = 2\mathbf{u}'\mathcal{L}^T(\mathbf{u})/R$  and orthogonality condition

$$\dot{\mathbf{R}}^T \cdot \dot{\mathbf{R}} = 4\mathbf{u}' \cdot \mathbf{u}'/R$$

Final equation of motion, with  $\mathbf{u} \cdot \mathbf{u} = R$ 

$$\mathbf{u}'' = \frac{1}{2}h\mathbf{u} + \frac{1}{2}R\mathcal{L}^T(\mathbf{u})\mathbf{F}_{kl}$$

Binding energy per unit reduced mass

$$h = [(2\mathbf{u}' \cdot \mathbf{u}' - (m_k + m_l)]/R$$

Rate of change from  $\hat{\mathbf{R}} \cdot \hat{\mathbf{R}}$ 

$$\frac{d}{dt} \left[ \frac{1}{2} \dot{\mathbf{R}}^2 - \frac{(m_k + m_l)}{R} \right] = \dot{\mathbf{R}} \cdot \mathbf{F}_{kl}$$

Conversion by  $h' = \mathbf{R}' \cdot \mathbf{F}_{kl}$  and  $\dot{\mathbf{R}}$ 

$$h' = 2\mathbf{u}' \cdot \mathcal{L}^T(\mathbf{u})\mathbf{F}_{kl}$$

Generalized  $4 \times 4$  matrix

$$\mathcal{L}(\mathbf{u}) = \begin{bmatrix} u_1 & -u_2 & -u_3 & u_4 \\ u_2 & u_1 & -u_4 & -u_3 \\ u_3 & u_4 & u_1 & u_2 \\ u_4 & -u_3 & u_2 & -u_1 \end{bmatrix}$$

Explicit components of  ${f R}$ 

$$R_1 = u_1^2 - u_2^2 - u_3^2 + u_4^2$$

$$R_2 = 2(u_1u_2 - u_3u_4)$$

$$R_3 = 2(u_1u_3 + u_2u_4)$$

$$R_4 = 0$$

Summing the squares and square root

$$R = u_1^2 + u_2^2 + u_3^2 + u_4^2$$

Case  $R_1 > 0$ : combine  $R_1$  and R

$$u_1^2 + u_4^2 = \frac{1}{2}(R_1 + R)$$

Redundancy  $u_4 = 0$ 

$$u_{1} = \left[\frac{1}{2}(R_{1} + R)\right]^{1/2}$$

$$u_{2} = \frac{1}{2}R_{2}/u_{1}$$

$$u_{3} = \frac{1}{2}R_{3}/u_{1}$$

Case  $R_1 < 0$ : subtract  $R_1$  from R

$$u_2^2 + u_3^2 = \frac{1}{2}(R - R_1)$$

Redundancy  $u_3 = 0$ 

$$u_{2} = \left[\frac{1}{2}(R - R_{1})\right]^{1/2}$$

$$u_{1} = \frac{1}{2}R_{2}/u_{2}$$

$$u_{4} = \frac{1}{2}R_{3}/u_{2}$$

Regularized velocity: invert  $\mathbf{R}'$  and use first property

$$\mathbf{u}' = \frac{1}{2} \mathcal{L}^T(\mathbf{u}) \mathbf{R}' / R = \frac{1}{2} \mathcal{L}^T(\mathbf{u}) \dot{\mathbf{R}}$$

Final equations of motion

$$\mathbf{u}'' = \frac{1}{2}h\,\mathbf{u} + \frac{1}{2}R\,\mathcal{L}^T\,\mathbf{F}_{kl}$$

$$h' = 2\,\mathbf{u}'\cdot\mathcal{L}^T\,\mathbf{F}_{kl}$$

$$t' = \mathbf{u}\cdot\mathbf{u}$$

Semi-major axis

$$a = -\frac{1}{2}(m_k + m_l)/h$$

Eccentricity:  $R = a(1 - e\cos\theta)$  and  $nt = \theta - e\sin\theta$ 

$$e^2 = (1 - R/a)^2 + 4(\mathbf{u} \cdot \mathbf{u}')^2 / [(m_k + m_l)a]$$

Bilinear relation:  $\dot{R}_4 = 0$ 

$$u_4u_1' - u_3u_2' + u_2u_3' - u_1u_4' = 0$$

# Unperturbed two-body motion

Maximum force:

$$j = \max_i (m_i/|\mathbf{r}_i - \mathbf{r}_{cm}|^2), \quad i = 1, N$$

Smallest inverse travel time

$$\beta_s = \mathbf{r}_s \cdot \dot{\mathbf{r}}_s / r_s^2, \qquad \mathbf{r}_s - \mathbf{r}_{cm} \Rightarrow \mathbf{r}_s$$

Perturber boundary

$$r_{\gamma} = R[2\tilde{m}/(m_b\gamma_{\min})]^{1/3}$$

Travel time:  $\dot{r}_s < 0$ 

$$\Delta t_{\rm in} = (r_s - r_\gamma)/|\dot{r}_s| \,,$$

Free-fall time

$$\Delta t_a = \left[2\Delta t_{\rm in}\dot{r}_s r_s^2/(m_b + m_s)\right]^{1/2}$$

Return time of dominant body

$$\Delta t_j = [2(r_j - r_\gamma)r_j^2/(m_b + m_j)]^{1/2}$$

Unperturbed time interval

$$\Delta t_{\gamma} = \min (\Delta t_{\rm in}, \Delta t_a, \Delta t_j, \Delta t_{cm})$$

Unperturbed periods

$$K = 1 + \frac{1}{2}\Delta t_{\gamma}/t_{K}$$

Final time interval

$$\Delta t = K \min (t_K, \Delta t_{\rm cm})$$

# KS algorithms

Perturber prediction

$$\mathbf{r}_{j} = \left( \left( \frac{1}{6} \mathbf{F}^{(1)} \, \delta t'_{j} + \frac{1}{2} \mathbf{F} \right) \delta t'_{j} + \mathbf{v}_{0} \right) \delta t'_{j} + \mathbf{r}_{0}$$

$$\dot{\mathbf{r}}_{j} = \left( \left( \frac{1}{2} \mathbf{F}^{(1)} \, \delta t'_{j} + \mathbf{F} \right) \delta t'_{j} + \mathbf{v}_{0}, \quad \delta t'_{j} = t - t_{j} \right)$$

KS prediction

 $\mathbf{u}$  and  $\mathbf{u}'$  to order  $\mathbf{u}^{(5)}$ 

Basic Hermite

Stabilization factor in  $\mathbf{u}''$ h predicted to order  $h^{(2)}$ 

KS transformations

Global coordinates and velocities  $\mathbf{r}_k, \mathbf{r}_l, \dot{\mathbf{r}}_k, \dot{\mathbf{r}}_l$ 

Physical perturbation

 ${f P}$  and  $\dot{{f P}}$  due to perturbers, set  ${f P}'=R\,\dot{{f P}}$  j>N: c.m. approximation or components

Slow-down factor

Include  $\kappa$  in **P** and  $\dot{\mathbf{P}}$ , also  $t' = \kappa \mathbf{u} \cdot \mathbf{u}$ 

Energy prediction (Stumpff method)

h to order  $h^{(4)}$ 

KS corrector

 $\mathbf{u}, \mathbf{u}'$  to order  $\mathbf{u}^{(5)}$  and h to  $h^{(4)}$ 

Time derivatives

Taylor series  $t'' = 2\mathbf{u} \cdot \mathbf{u}', \dots, t^{(6)} = 2\mathbf{u} \cdot \mathbf{u}^{(5)} + \dots$ 

#### Hermite KS

Standard KS

$$\mathbf{u}'' = \frac{1}{2}h\,\mathbf{u} + \frac{1}{2}R\,\mathcal{L}^T\,\mathbf{F}_{kl}$$

$$h' = 2\,\mathbf{u}'\cdot\mathcal{L}^T\,\mathbf{F}_{kl}$$

$$t' = \mathbf{u}\cdot\mathbf{u}$$

New notation

$$\mathbf{F}_{\mathbf{u}} = \mathbf{u}''$$

$$\mathbf{Q} = \mathcal{L}^T \mathbf{P},$$

with  $\mathbf{P} = \mathbf{F}_{kl}$  as the perturbing force.

Basic equations

$$\mathbf{F}_{\mathbf{u}} = \frac{1}{2}h\,\mathbf{u} + \frac{1}{2}R\,\mathbf{Q}$$

$$h' = 2\,\mathbf{u}'\cdot\mathbf{Q}$$

$$t' = \mathbf{u}\cdot\mathbf{u}$$

Hermite  $\mathbf{F}$ ,  $\mathbf{F'}$  formulation

$$\mathbf{F}_{\mathbf{u}} = \frac{1}{2}h\,\mathbf{u} + \frac{1}{2}R\,\mathbf{Q}$$

$$\mathbf{F}'_{\mathbf{u}} = \frac{1}{2}(h'\mathbf{u} + h\mathbf{u}' + R'\mathbf{Q} + R\mathbf{Q}')$$

$$h' = 2\,\mathbf{u}'\cdot\mathbf{Q}$$

$$h'' = 2\mathbf{F}_{\mathbf{u}}\cdot\mathbf{Q} + 2\mathbf{u}'\cdot\mathbf{Q}'$$

$$t' = \mathbf{u}\cdot\mathbf{u}$$

The derivatives of  $\mathbf{P}$ ,  $\mathbf{Q}$  and t' are readily available. Note that  $\mathbf{P}' = R\dot{\mathbf{P}}$  and that  $\mathcal{L}^T(\mathbf{u}')$  can be obtained by substituting  $\mathbf{u}'$  for  $\mathbf{u}$ . For implementation, significant accuracy can be gained by high-order prediction (not used in standard Hermite).

## N-body interface

Centre of mass acceleration

$$\ddot{\mathbf{r}}_{cm} = (m_k \mathbf{F}_k + m_l \mathbf{F}_l) / (m_k + m_l)$$

Global coordinates

$$\mathbf{r}_k = \mathbf{r}_{cm} + \mu \mathbf{R}/m_k$$
 $\mathbf{r}_l = \mathbf{r}_{cm} - \mu \mathbf{R}/m_l$ 

Relative perturbation

$$\gamma = |\mathbf{F}_k - \mathbf{F}_l|R^2/(m_k + m_l)$$

Tidal approximation

$$r_{\gamma} = R[2\tilde{m}/(m_k + m_l)\gamma_{\min}]^{1/3}, \qquad \gamma_{\min} \simeq 10^{-6}$$

Perturber selection

$$r_{ij} < r_{\gamma}, \qquad R = a(1+e)$$

Regularized time-step

$$\Delta \tau = \eta_u (1/2|h|)^{1/2} 1/(1+1000\gamma)^{1/3}$$

Physical time-step

$$\Delta t = \sum_{k=1}^{n} \frac{1}{k!} t_0^{(k)} \Delta \tau^k, \qquad n = 6$$

Time derivatives

$$t_0'' = 2\mathbf{u}' \cdot \mathbf{u}$$
  
 $t_0^{(3)} = 2\mathbf{u}'' \cdot \mathbf{u} + 2\mathbf{u}' \cdot \mathbf{u}$